THREE-DIMENSIONAL MODEL OF A COMPLEX BETWEEN A Fc EPSILON RECEPTOR ALPHA CHAIN AND A Fc REGION OF AN IgE ANTIBODY AND USES THEREOF

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CROSS-REFERENCE TO RELATED APPLICATION

This Application claims priority to provisional application U.S. Serial No. 60/189,853, filed March 15, 2000, "THREE-DIMENSIONAL MODEL OF A COMPLEX BETWEEN A Fc EPSILON RECEPTOR ALPHA CHAIN AND A Fc REGION OF AN IgE ANTIBODY AND USES THEREOF."

FIELD OF THE INVENTION

The present invention relates to a crystal and a three-dimensional (3-D) model of a complex between a Fc epsilon receptor alpha chain (FcεRIα, or FceRIa) protein and a constant region of an IgE antibody that includes the Cε3 and Cε4 domains (Fc-Cε3/Cε4, or Fc-Ce3/Ce4, region). The present invention also relates to the use of that model to produce muteins and inhibitors useful in the diagnosis and treatment of allergy and the regulation of other immune responses in an animal.

BACKGROUND OF THE INVENTION

Antibody Fc-receptors (FcRs) play an important role in the immune response by coupling the specificity of secreted antibodies to a variety of cells of the immune system. A number of cell types, including macrophages, mast cells, eosinophils, and basophils, express membrane-bound FcRs at their surfaces. The binding of antibodies to FcRs

provides antigen-specificity to these cells, which upon activation release further cell-specific mediators of the immune response, such as interleukins, initiators of inflammation, leukotrienes, prostaglandins, histamines, or cytotoxic proteins. The adoptive specificity of the FcRs allows a combinatorial approach to pathogen elimination, by coupling the diversity of antibody antigen-recognition sites to the variety of cell-types expressing these receptors.

FcR-initiated mechanisms are important in normal immunity to infectious disease as well as in allergies, antibody-mediated tumor recognition, autoimmune diseases, and other diseases in which immune responses are abnormal (i.e., not regulated). Recent experiments with transgenic mice have demonstrated that the FcRs control key steps in the immune response, including antibody-directed cellular cytotoxicity and inflammatory cascades associated with the formation of immune complexes; see, for example, Ravetch et al., 1998, *Annu Rev Immunolo 16*, 421-432. Receptors that bind IgG (FcgRI, FcgRII, and FcgRIII, known collectively as FcgRs) mediate a variety of inflammatory reactions, regulate B-cell activation, and also trigger hypersensitivity reactions. The high affinity Fc epsilon receptor (also known as the IgE receptor or FceRI) is associated with the activation of mast cells and the triggering of allergic reactions and anaphylactic shock. Knockout mice for the FceRI alpha chain (FcεRIα) are unable to mount IgE-mediated anaphylaxis (see for example, Dombrowicz et al., 1993, *Cell 75*, 969-976), although FcgRs are still able to activate mast cells (see, for example, Dombrowicz et al., 1997, *J. Clin. Invest. 99*, 915-925; Oettgen et al., 1994, *Nature 370*, 367-370). FceRI has also been shown to trigger anti-parasitic reactions from platelets and eosinophils as well as

deliver antigen into the MHC class II presentation pathway for the activation of T cells; see, for example, Gounni et al., 1994, *Nature 367*, 183-186; Joseph et al., 1997, *Eur. J. Immunol. 27*, 2212-2218; Maurer et al., 1998, *J. Immunol. 161*, 2731-2739. The beta subunit of FceRI has been associated with asthma in genetic studies; see, for example, Hill et al., 1996, *Hum. Mol. Genet. 5*, 959-962; Hill et al., 1995, *Bmj 311*, 776-779; Kim et al., 1998, *Curr. Opin. Pulm. Med. 4*, 46-48; Mao et al., 1998, *Clin. Genet. 53*, 54-56; Shirakawa et al., 1994, *Nat. Genet. 7*, 125-129. A significant fraction of the population (~20%) may be affected by allergies, and this century has seen a substantial increase in asthma. Since IgE binding to FceRI is a requisite event in the reaction to different allergens, therapeutic strategies aimed at inhibiting FceRI could provide a useful treatment for these diseases. For example, monoclonal antibodies that target IgE and block receptor binding have shown therapeutic potential; see, for example, Heusser et al., 1997, *Curr. Opin. Immunol. 9*, 805-813.

FceRI is found as a tetrameric (abg_2) or trimeric (ag_2) membrane bound receptor on the surface of mast cells, basophils, eosinophils, langerhans cells and platelets. The alpha chain, also referred to as FcεRIα, of FceRI binds IgE molecules with high affinity (K_D of about 10^{-9} to 10^{-10} moles/liter (M)), and can be secreted as a 172-amino acid soluble, IgE-binding fragment by the introduction of a stop codon before the single C-terminal transmembrane anchor; see, for example, Blank et al.,1991, *E. J. Biol. Chem. 266*, 2639-2646, which describes the secretion of a soluble IgE-binding fragment of 172 amino acids. The extracellular domains of the human FcεRIα protein belong to the immunoglobulin (Ig) superfamily and contain seven N-linked glycosylation sites.

Glycosylation of FcεRIα affects the secretion and stability of the receptor, but is not required for IgE-binding; see, for example, LaCroix et al., 1993, *Mol. Immunol. 30*, 321-330; Letourneur et al.,1995, *J. Biol. Chem. 270*, 8249-8256; Robertson, 1993, *J. Biol. Chem. 268*, 12736-12743; Scarselli et al., 1993, *FEBS Lett 329*, 223-226. The beta and gamma chains of FceRI are signal transduction modules.

Prior investigators have disclosed the nucleic acid sequence for human FcεRIα; see, for example, U.S. Patent No. 4,962,035, by Leder, issued October 9, 1990; U.S. Patent No. 5,639,660, by Kinet et al., issued June 17, 1997; Kochan et al., 1988, *Nucleic Acids Res. 16*, 3584; Shimizu et al., 1988, *Proc. Natl. Acad. Sci. USA 85*, 1907-1911; and Pang et al., 1993, *J. Immunol. 151*, 6166-6174. Nucleic acid sequences have also been reported for the human FceRI beta and gamma chains; see, respectively, Kuster et al., 1992, *J. Biol. Chem. 267*, 12782-12787; Kuster et al., 1990, *J. Biol. Chem. 265*, 6448-6452. Nucleic acid sequences have also been reported for nucleic acid molecules encoding canine FcεRIα, murine FcεRIα, rat FcεRIα, feline FcεRIα and equine FcεRIα proteins; see, respectively, GenBank™ accession number D16413; Swiss-Prot accession number P20489 (represents encoded protein sequence); GenBank accession number J03606; PCT Publication No. WO 98/27208, by Frank et al., published June 25, 1998, referred to herein as WO 98/27208; and PCT Publication No. WO 99/38974, by Weber et al., published August 5, 1999, referred to herein as WO 99/38974. In addition, methods to detect IgE antibodies using a FcεRIα protein have been reported in PCT Publication No. WO 98/23964, by Frank et al., published June 4, 1998, referred to herein as WO 98/23964; WO 98/27208, *ibid.*; PCT Publication No. WO 98/45707, by

Frank et al., published October 15, 1998, referred to herein as WO 98/45707; and WO 99/38974, *ibid.*. WO 98/23964, WO 98/27208, WO 98/45707 and WO 99/38974 are each incorporated by reference herein in its entirety.

There have been several reports of the use of mutagenesis and swapping techniques to attempt to identify amino acids of either FcεRIα or IgE involved in the binding of (i.e., interaction between) those respective proteins, reports attempting to model FcεRIα proteins based on homology to other Ig-superfamily members, and reports that identify compounds that apparently inhibit such binding; see, for example, Cook et al., 1997, *Biochemistry 36*, 15579-15588; Hulett et al., 1994, *J. Biol. Chem. 269*, 15287-15293; Hulett et al., 1995, *J. Biol. Chem 270*, 21188-21194; Mallamaci et al., 1993, *J. Biol. Chem. 268*, 22076-22083; Robertson, 1993, *ibid.*; Scarselli et al., 1993, *ibid.* McDonnell et al., 1997, *Biochem. Soc. Trans. 25*, 387-392; McDonnell et al., 1996, *Nat. Struc. Biol. 3*, 419-426; PCT Publication No. WO 97/40033, by Cheng et al., published October 30, 1997; U.S. Patent No. 5,180,805, by Gould et al, issued January 19, 1993; U.S. Patent No. 5,693,758, by Gould et al., issued December 2, 1997; PCT Publication No. WO 96/01643, by Gould et al., published January 25, 1996; PCT Publication No. WO 95/14779, by Gould et al., published June 1, 1995. None of these references, however, describe isolated crystals of FcεRIα proteins or 3-D models derived from crystals.

Despite what is known about FcRs and their interaction with antibodies, there remains a need for FcRs and antibodies with improved characteristics, such as enhanced affinity for their ligands, altered substrate specificity, increased stability, and increased

solubility for use in diagnosis, treatment and prevention of allergy and other abnormal immune responses. Also needed for safe and efficacious compounds to prevent or treat allergy and to regulate other immune responses in an animal.

SUMMARY OF THE INVENTION

The present invention includes isolated crystals of a complex between the extracellular domains of antibody receptor proteins (FcRs) and constant regions (Fc regions) of antibodies, three-dimensional (3-D) models of such crystals and modifications of such models. The present invention also includes compounds that inhibit the ability of FcRs to bind to antibodies as well as FcR muteins and other modified FcRs as well as antibody muteins and other modified antibodies. Also included in the present invention are methods to produce and use such crystals, models, inhibitory compounds, muteins, and other modified proteins. As such, the present invention includes FcRs and antibodies with improved functions such as increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility, including but not limited to reduced aggregation. Such proteins, also referred to as muteins, are useful to detect allergy and other immune response abnormalities as well as to protect an animal from such abnormalities. The present invention also provides safe and efficacious inhibitory compounds to protect (e.g., prevent, treat, reduce the consequences of) an animal from allergy and to regulate other immune responses in an animal.

The present invention includes a 3-D model of a complex between an extracellular domain of a human high affinity Fc epsilon receptor alpha chain (FcεRIα) protein and a human IgE Fc region comprising Cε3 and Cε4 domains, wherein the model substantially

represents the atomic coordinates specified in Table 1. The present invention also includes a 3-D model comprising a modification of a model substantially representing the atomic coordinates specified in Table 1. Also included in the present invention are methods to produce such models.

The present invention also includes an isolated crystal of a complex between an extracellular domain of a human high affinity Fc epsilon receptor alpha chain protein and a human IgE Fc region comprising Cε3 and Cε4 domains.

The present invention includes a method to identify a compound that inhibits the binding between an IgE antibody and a FcεRIα protein. The method includes the step of using a 3-D model of the present invention, and particularly one substantially represents the atomic coordinates specified in Table 1. Also included in the present invention are inhibitory compounds identified using such a method. Also included are therapeutic compositions that include such inhibitory compounds and methods to use such therapeutic compositions to protect an animal from allergy or to regulate other immune responses (e.g., protect an animal from other abnormal immune responses).

The present invention also includes a mutein that binds to a Fc domain of an antibody or to a Fc binding domain of a FcR. Such a mutein has an improved function compared to a protein that includes SEQ ID NO:2 or SEQ ID NO:6, respectively. Examples of such an improved function include increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, decreased aggregation, and increased solubility. Such a mutein is produced by a method that includes the following steps: (a) analyzing a 3-D model substantially representing the atomic coordinates

specified in Table 1 to identify at least one amino acid of the protein represented by the model which if replaced by a specified amino acid would effect an improved function of the protein; and (b) replacing the identified amino acid(s) to produce the mutein having such an improved function. The present invention also includes a mutein having an improved function compared to an unmodified FcεRIα protein or IgE Fc region.

Also included are muteins that are chemically modified FcεRIα proteins or antibodies. Also included are nucleic acid molecules that encode muteins of the present invention, recombinant molecules and recombinant cells including such nucleic acid molecules and methods to produce such muteins. Also included are diagnostic reagents and diagnostic kits including such muteins, therapeutic compositions including such muteins, and methods to detect or protect an animal from allergy or other abnormal immune responses.

The present invention also includes a method to improve a function of a FcεRIα protein or IgE Fc region which includes the steps of: (a) analyzing a 3-D model substantially representing the atomic coordinates specified in Table 1 to identify at least one amino acid of the protein which if replaced by a specified amino acid improves at least one of the functions of the protein; and (b) replacing the identified amino acid(s) to produce a mutein having at least one of the improved functions.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig.1 shows an electron density map and ribbon diagrams depicting the overall structure of the IgE-Fc:FcεRIα complex. Fig. 1a shows a stereo diagram from a σ_a-weighted $2F_o$-F_c simulated annealing omit electron density map at 3.5 angstroms. The

complex is contoured at 1.25σ. FcεRIα residues 129-136 of FcεRIα and IgE-Fc loop residues 334-336 and 362-364 are shown. Fig. 1b is a side view of the IgE-Fc:FcεRIα complex depicting the two Fc chains (yellow and red ribbon, upper left of figure) and the FcεRIα chain (blue ribbon, lower right of figure). Binding sites 1 and 2 are indicated. The cell membrane would lie below the receptor. Fig. 1c is a top view of the IgE-Fc:FcεRIα complex shown in Fig. 1b.

Fig. 2 shows a surface representation of the IgE-Fc:FcεRIα complex. Fig. 2a is a side view of the IgE-Fc:FcεRIα complex highlighting how the convex surface of the receptor interacts asymmetrically with the two IgE-Fc Cε3 domains. The two Fc chains are in yellow and red while the FcεRIα chain is in blue. Carbohydrate surfaces are white, detergent surface is black. Fig. 2b is a top view of the IgE-Fc:FcεRIα complex surface representation shown in Fig. 2a. Fig. 2c is a superposition of the two IgE-Fc Cε3 domains . The twofold symmetry of the IgE-Fc domains is broken in the Cε2-Cε3 linker region (residues 328-336) by interactions with the receptor. Superposition of the Cε3 domains leads to a small displacement in the Cε4 domain, because of a 3° difference in Cε3 and Cε4 pseudo-dyad axes. Fig. 2d is a surface representation of both IgE-Fc and FcεRIα in which the IgE-Fc:FcεRIα complex has been separated to expose the surfaces involved in binding. The IgE (upper left) is oriented to give an end-on view of the Cε3 domains. Binding residues that bind FcεRIα are shown in yellow (Site 1) and red (Site 2). A top and side view of the FcεRIα is shown on the right-hand side of Fig. 2d. Residue Y131 of site 1 and the binding pocket for P426 of the IgE-Fc are labeled. Carbohydrate is shown in grey.

Fig. 3 details the interactions in the IgE-Fc:FcεRIα complex at Site 1 and Site 2. Fig. 3a is a plot showing the buried surface area of residues in the IgE-Fcε3 domains. The top half of the graph shows residues buried in the Site 1 interaction (yellow bars), while the bottom half of the graph shows residues buried in the Site 2 interaction (red bars). The IgE loops are identified above the plot. 50 Å of buried surface area of N394 is due to attached carbohydrate. Fig. 3b is a stick model diagram of residue interactions at Site 1. The IgE-Fc and FcIα chains are tan and blue, respectively. Binding loops are labeled at their termini, side chains of residues buried in the complex are shown and Y131 is labeled. Fig. 3c is a stick model diagram of the residue interactions at Site 2. The IgE-Fc and FcεRIα chains are red and blue, respectively. Side chains of residues buried in the complex are shown. Fig. 3d is a space filling model showing binding of CHAPS detergent molecule in the IgE-Fc:FcεRIα complex. Atoms less than 4Å apart have dotted lines between them and the residues are labeled. No density appears for the flexible top-end of the detergent and those atoms are not labeled.

Fig. 4 illustrates the conservation of amino-acid residues and contacts at the IgE-Fc:FcεRIα interfaces in IgG receptors and antibodies. Contacting residues are defines as interatomic distances <4 Å. Fig. 4a shows the Site 1 interacting residues and their conservation in related human receptors and antibodies. Absolutely conserved residues are highlighted in bold and partially conserved residues are lightly highlighted (yellow for IgE, blue for FcεRIα). Dark lines are drawn for residues making the largest number of contacts across the interface, lighter lines for intermediate number of contacts, and dashed lines for the fewest contacts. Fig. 4b shows the Site 2 interacting residues and their

conservation in human related Fc receptors and antibodies. Receptor residues are highlighted in blue, antibody residues in red. Three residues in IgG2 (PVA) that disrupt binding to FcγRI are boxed in black. Fig. 4c is a closeup of the Site 2 trp/proline interaction (FcR surface with IgE-ribbon interaction). Also shown are residues implicated in the IgG specificity between different receptor subtypes (corresponding to residues 332-334 in IgE) that interact with the FG loop. Fig. 4d is shows how FcRY131 in Site 1 interacts with a shallow pocket on the Cε3 domain that could be a source of specificity for IgG interactions (Y changes to H or R in FcγRII and FcγRIII).

Fig. 5 depicts a kinetic scheme for the binding of IgE to its receptor. The interaction of each Cε3 domain with distinct surfaces of the FcεRIα structure suggests a kinetic scheme in which transient release of one of the Cε3 domains may occur within the complex. This could lead to two distinct pathways for the association and dissociation of the complex, consistent with the experimental observation of two distinct off-rates . Transient opening of the complex may allow inhibitors to enhance the dissociation of receptor-bound IgE by preventing the re-binding of an exposed Cε3 domain within the complex.

Fig. 6 is a ribbon-model showing the superposition of the Fc portion of an intact IgG antibody (1IGY)27 and IgG Fc receptor FcγRII22 onto the IgE-Fc:FcεRIα complex. The IgE complex is shown in beige and the IgG homologues in blue. Only a minor adjustment of the other IgG domain is required to fit the IgE complex.

Fig. 7 shows a hypothetical model for an intact IgE:Fc receptor complex. The Fc chains are in red and yellow, the FcεRIα chain is in blue. Antibody Fab regions are shown in beige.

DETAILED DESCRIPTION OF THE INVENTION

The present invention includes isolated crystals of complexes between the extracellular domains of FcRs and Fc regions of antibodies, 3-D models of such crystals and modifications of such models. The present invention also includes compounds that inhibit the ability of FcRs to bind to antibodies as well as muteins and other modified FcRs and antibodies. Also included in the present invention are methods to produce and use such crystals, models, inhibitory compounds, muteins, and other modified proteins.

The present invention includes an isolated crystal of a complex between an extracellular domain of a high affinity Fc epsilon receptor alpha chain (FcεRIα) and a Fc region comprising the Cε3 and Cε4 domains of an IgE antibody (Fc-Cε3/Cε4), a 3-D model of such a crystal and a modification of such a model. As used herein, the term "a" entity or "an" entity refers to one or more of that entity; for example, a crystal or a model refers to one or more crystals or models, respectively. As such, the terms "a" (or "an"), "one or more" and "at least one" can be used interchangeably herein. It is also to be noted that the terms "comprising", "including", and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of" refers to one or more of the compounds in the list that follows, including mixtures, or combinations, of two or more of the compounds.

As used herein, an extracellular domain of a FcεRIα protein is the portion of the FceRI alpha chain that is exposed to the environment outside the cell and that binds to the Fc domain of an IgE antibody. Such an extracellular domain can be (a) a complete extracellular domain which is a domain that extends from the first amino acid of a mature FceRI alpha chain through the last amino acid prior to the start of the transmembrane region or a domain that is functionally equivalent, in that such a domain includes a D1 and D2 domain, displays a similar affinity for the IgE antibody to which such an FcεRIα protein naturally binds, and produces crystals having sufficient quality to enable structure determination, or (b) a fragment of any of the extracellular domains of (a), wherein the fragment retains its ability to bind to the Fc domain of an antibody. As used herein, the terms binding to an antibody and binding to the Fc domain (i.e., constant region) of an antibody can be used interchangeably since it is recognized that a FcR binds to the Fc domain of an antibody. A FcR (i.e., a protein that can bind to an antibody), such as a FcεRIα protein, can be a full-length FcR (e.g., a full-length FceRI alpha chain), or any fragment thereof, wherein the fragment binds to an antibody. Similarly an antibody, or an Fc region thereof, can be a full-length antibody, or full-length Fc region thereof, or any fragment thereof that binds to a FcR. In one embodiment an Fc region comprises Cε3 and Cε4 domains. Preferably a FcR binds to an antibody with an affinity (K_A) of at least about 10^8 liters/mole (M^{-1}), more preferably of at least about $10^9 M^{-1}$, and even more preferably of at least about $10^{10} M^{-1}$.

The present invention is surprising in several aspects. For example, this is the first report of an isolated crystal of a complex between an extracellular domain of a

FcεRIα protein and a Fc-Cε3/Cε4 region of an IgE antibody, and in particular of an isolated crystal of sufficient quality that a crystal structure, i.e., a 3-D model, could be derived therefrom. Generation of such a crystal was very difficult and non-obvious and has been attempted by others without success. The inventors tried many approaches before discovering a preferred FcεRIα protein and a preferred Fc-Cε3/Cε4 region from which to make a useful crystal. Part of the reason for the difficulty is that the FcεRIα protein is highly glycosylated. Although crystals could be produced using a FcεRIα protein that consists of amino acids 1 through 176 of the mature human FcεRIα protein, a protein that is denoted herein as PhFcεRIα$_{1\text{-}176}$, or the hFcεRIα$_{1\text{-}176}$ protein, and has an amino acid sequence denoted herein as SEQ ID NO:2, much better crystals could be generated using a FcεRIα protein that consists of amino acids 1 through 176 of the mature human FcεRIα protein that had been mutated to replace four N-linked glycosylation sites with other amino acids at positions 74, 135, 142 and 143 of SEQ ID NO:2 to produce a protein having SEQ ID NO:4, the protein being denoted herein as PhFcεRIα$_{1\text{-}176mut}$, or the hFcεRIα$_{1\text{-}176mut}$ protein. An example of a nucleic acid molecule encoding PhFcεRIα$_{1\text{-}176}$ is referred to herein as nhFcεRIα$_{1\text{-}528}$, the nucleic acid sequence of which is denoted herein as SEQ ID NO:1. An example of a nucleic acid molecule encoding PhFcεRIα$_{1\text{-}176mut}$ is referred to herein as nhFcεRIα$_{1\text{-}528mut}$, the nucleic acid sequence of which is denoted herein as SEQ ID NO:3. Identification of an appropriate Fc-Cε3/Cε4 region to crystallize was also difficult. The first such region to be used successfully is referred to herein as PhFc-Cε3/Cε4$_{1\text{-}222}$ which is composed of the four amino acids alanine, aspartic acid, proline and cysteine at the amino terminus followed by amino acids 330 through547 of the human

IgE Fc constant region, using the numbering system of Dorrington et al, 1978, *Immunol Rev 41*, 3-25. PhFc-Cε3/Cε4$_{1\text{-}222}$ is represented herein by SEQ ID NO:6. An example of a nucleic acid molecule encoding PhFc-Cε3/Cε4$_{1\text{-}222}$ is referred to herein as nhFc-Cε3/Cε4$_{1\text{-}666}$, the nucleic acid sequence of which is referred to herein as SEQ ID NO:5. It was also discovered that better crystals are generated when PhFcεRIα$_{1\text{-}176}$ and PhFc-Cε3/Cε4$_{1\text{-}222}$ are produced in insect cells, using a method such as that described in the Examples.

Determination of the crystal structure of the complex between PhFcεRIα$_{1\text{-}176mut}$ and PhFc-Cε3/Cε4$_{1\text{-}222}$, each produced in *Trichoplusia ni* (Hi-5) cells, resulted in a 3-D model that substantially represents the atomic coordinates specified in Table 1. Amino acids are represented herein by their standard three or one letter codes; see, for example, Sambrook et al., *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Labs Press, 1989, which is incorporated herein by reference in its entirety. Prior to obtaining a crystal of sufficient quality to solve its crystal structure using insect-cell produced PhFcεRIα$_{1\text{-}176mut}$ and PhFc-Cε3/Cε4$_{1\text{-}222}$, a number of other proteins were tried without success, as described in the Examples. , including a FcεRIα protein spanning from amino acid 1 through 171 of SEQ ID NO:2 produced in *Pichia pastoris*, and FcεRIα proteins spanning from amino acid 1 through 172 of SEQ ID NO:2 produced in Chinese hamster ovary cells, *Trichoplusia ni* cells, and *Spodoptera frugiperda* cells without success. Without being bound by theory, it is believed that PhFcεRIα$_{1\text{-}176mut}$ was a better candidate because it apparently represents a complete extracellular domain and it lacked carbohydrates that interfered with complex formation for structural analysis.

The 3-D model of the complex between PhFcεRIα$_{1\text{-}176mut}$ and PhFc-Cε3/Cε4$_{1\text{-}222}$ is also very surprising in view not only of the knowledge of the structure of proteins containing immunoglobulin domains, herein also referred to as Ig domains, but also in view of the crystal structures of FcεRIα alone, which is disclosed in U.S. Patent Application Serial No. 09/434,193, filed November 4, 1999, by Jardetzky et al., and in PCT Publication No. WO 00/26246, published May 11, 2000, by Jardetzky et al., and of Fc-Cε3/Cε4 alone, which is disclosed in U.S. Patent Application Serial No. 60/189,403, filed March 15, 2000, by Jardetzky et al. WO 00/26246, *ibid.*, 09/434,193, *ibid.*, and 60/189,403, *ibid.* are incorporated by reference herein in their entireties. Not only is the structure of FcεRIα in the complex fairly similar to the unique structure of FcεRIα alone, but, even more surprisingly, the structure of Fc-Cε3/Cε4 in the complex is very different from that of Fc-Cε3/Cε4 alone. For example, as disclosed in 60/189,403, *ibid.*, the Fc region of IgE alone exists in a closed conformation whereas receptor-bound IgE Fc exists in an open conformation. The model also predicts that a FcεRIα protein and an IgE Fc region bind at a stoichiometry of 1:1 which is surprising since each Fc region has two Cε3 domains. Comparison of these structural similarities and differences are described in greater detail in the Examples. Analysis of the model which substantially represents the atomic coordinates specified in Table 1 indicates the necessity of such a model for proper interpretation and refinement of mutagenesis and region swapping studies that have been reported. Such a model permits differentiation, even more so than models of FcεRIα alone as disclosed in 09/434,193, *ibid.*, WO 00/26246, *ibid.*, and Garman et al., 1999, *Cell 95*, 951-961, between amino acids directly or indirectly influencing binding of IgE to

FcεRIα and demonstrates where amino acids and amino acid segments identified in mutagenesis and swapping studies are positioned on the protein. By using a model of the present invention one can identify the interactions of FcεRIα and IgE, thereby identifying amino acids to target for mutein production or regions to target for the development of compounds to inhibit binding of IgE to its receptor. Such a model can be used alone or in conjunction with a model of FcεRIα alone (09/434,193, *ibid.* or WO 00/26246, *ibid.*) or Fc-Cε3/Cε4 alone (60/189,403, *ibid.*).

One embodiment of the present invention is an isolated crystal of a complex between an extracellular domain of a FcεRIα protein and a Fc-Cε3/Cε4 region of an IgE antibody. As used herein, an isolated crystal is a crystal of a protein that has been produced in a laboratory; that is, an isolated crystal is produced by an individual and is not an object found *in situ* in nature. It is appreciated by those skilled in the art that there are a variety of techniques to produce crystals including, but not limited to, vapor diffusion using a hanging or sitting drop methodology, vapor diffusion under oil, and batch methods; see, for example, Ducruix et al., eds., 1991, *Crystallization of nucleic acids and proteins; A practical approach*, Oxford University Press, and Wyckoff et al., eds., 1985, *Methods in Enzymology 11*, 49-185; each reference is incorporated by reference herein in its entirety. It is also to be appreciated that crystallization conditions can be adjusted depending on a protein's inherent characteristics as well as on a protein's concentration in a solution and that a variety of precipitants can be added to a protein solution in order to effect crystallization; such precipitants are known to those skilled in the art. In a preferred embodiment, a crystal of a complex between an FcεRIα protein and

a Fc-Cε3/Cε4 region is produced in a solution by adding a precipitant such as polyethylene glycol (PEG) or PEG monomethylether. In one embodiment, a crystal of the present invention is produced in the presence of 3-[3-(cholamidopropyl) dimethylammonio]-1-propane-sulfonate (CHAPS), or a similar detergent. It is also to be noted that a FcεRIα protein and Fc-Cε3/CCε4 region used to produce a crystal can be produced by a variety of methods, including purification of a native protein, chemical synthesis of a protein, or recombinant production of a protein. Although a number of cell types can be used to recombinantly produce such a protein, insect cells, such as, but not limited to *Trichoplusia ni* and *Spodoptera frugiperda*, are preferred, with *Trichoplusia ni* cells being more preferred. Additional methods to produce proteins are disclosed below.

Isolated crystals of the present invention can include heavy atom derivatives, such as, but not limited to, gold, platinum, mercury, selenium, copper, and lead. Such heavy atoms can be introduced randomly or introduced in a manner based on knowledge of 3-D models of the present invention. Additional crystals of the present invention are not derivatized. In one embodiment, an isolated crystal of the present invention is a co-crystal of a FcεRIα protein bound to a Fc domain of an IgE antibody in the presence of a compound that inhibits the binding of a FcεRIα protein to a Fc domain of an IgE antibody. Additional crystals of the present invention include crystals produced from proteins that are muteins of the present invention or other proteins that are represented by a 3-D model of the present invention.

An isolated crystal of the present invention can be the crystal of a complex between any suitable extracellular domain of a FcεRIα protein and a Fc region that binds

to FcεRIα, such as a Fc comprising Cε3 domains or a Fc comprising Cε3 and Cε4 domains. Suitable FcεRIα proteins include mammalian FcεRIα proteins, with human, canine, feline, equine, rat and murine FcεRIα proteins being preferred, and human FcεRIα proteins being even more preferred. Suitable Fc-Cε3/Cε4 regions include mammalian Fc-Cε3/Cε4 regions, proteins, with human, canine, feline, equine, rat and murine Fc-Cε3/Cε4 regions being preferred, and human Fc-Cε3/Cε4 regions being even more preferred. A preferred crystal of the present invention diffracts X-rays to a resolution of about 4.5 angstroms or higher (i.e., lower number meaning higher resolution), with resolutions of about 4.0 angstroms or higher, about 3.5 angstroms or higher, about 3.25 angstroms or higher, about 3 angstroms or higher, about 2.5 angstroms or higher, about 2 angstroms or higher, about 1.5 angstroms or higher, and about 1 angstrom or higher being increasingly more preferred. It is appreciated, however, that additional crystals of lower resolutions can have utility in discerning overall topology of the structures, e.g., location of a binding site or where a molecule binds to a receptor or to an antibody. A particularly preferred isolated crystal of the present invention has the amino acid sequence SEQ ID NO:2, amino acid sequence SEQ ID NO:4, or a sequence essentially equivalent that represents an extracellular domain of another mammalian FcεRIα protein in complex with a Fc-Cε3/Cε4 region having amino acid sequence SEQ ID NO:6, or a sequence essentially equivalent that represents another mammalian Fc-Cε3/Cε4 region. Preferred are crystals that belong to spacegroup $P4_12_12$ or spacegroup R32. Particularly preferred crystals include: a crystal belonging to spacegroup $P4_12_12$ that has cell dimensions of 126 angstroms x 126 angstroms x 129 angstroms and that diffracts

X-rays to a resolution of about 4.5 angstroms; and a crystal belonging to spacegroup R32 that has cell dimensions of 192.8 angstroms x 192.8 angstroms x 302 angstroms and that diffracts X-rays to a resolution of about 3.25 angstroms.

The present invention includes a 3-D model of a complex between an extracellular domain of a FcεRIα protein and a Fc-Cε3/Cε4 region that substantially represents the atomic coordinates specified in Table 1. The present invention also includes 3-D models that comprise modifications of the model substantially represented by the atomic coordinates specified in Table 1. Each such modification represents a complex between a Fc receptor protein that binds to a Fc domain of an antibody and an antibody Fc region that binds to a Fc receptor protein. A 3-D model of a complex between an extracellular domain of a FcεRIα protein and a Fc-Cε3/Cε4 region is a representation, or image, that predicts the actual structure of the corresponding complex. As such, a 3-D model is a tool that can be used to probe the relationship between the complex's structure and function at the atomic level and to design muteins (i.e., genetically and/or chemically altered FcRs or antibodies) having an improved function, such as, but not limited to: increased (i.e., enhanced) stability; increased antibody or FcR, respectively, binding activity, for example, by, increasing the affinity for an antibody or FcR, respectively, by, for example, increasing the association rate and/or decreasing the dissociation rate between a FcR and an antibody or by altering substrate specificity (e.g., enhancing the ability of a FcR of a certain species and class to bind to antibody from another species and/or another antibody class); and/or increased solubility (e.g., reduced aggregation). It is well known to those skilled in the art, however, that a 3-D model of a protein or a

complex derived by analysis of protein or complex crystals is not identical to the inherent structure of the protein or complex. See, for example, Branden et al., *Introduction to Protein Structure*, Garland Publishing Inc., New York and London, 1991, especially on page 277, which states "not surprisingly the model never corresponds precisely to the actual crystal." Furthermore, the model can be subjected to further refinements to more closely correspond to the actual structure of a complex between a FcR and antibody. Such a refined model, which is an example of a modification of the present invention, is a better predictor of the actual structure and mechanism of action of the complex that the model represents. A refinement of a 3-D model of the present invention refers to an improved model of a complex between an extracellular domain of a FcεRIα protein and a Fc-Cε3/Cε4 region that can be obtained in a variety of ways known to those skilled in the art. Refinements can include models determined to more preferred degrees of resolution, preferably to about 4.5 angstroms, more preferably to about 4 angstroms, more preferably to about 3.5 angstroms, more preferably to about 3.25 angstroms, more preferably to about 3 angstroms, more preferably to about 2.5 angstroms, more preferably to about 2 angstroms, more preferably to about 1.5 angstroms, and even more preferably to about 1 angstrom. Preferred refinements are obtained using the 3-D model as a basis for such improvements.

One embodiment of the present invention is a 3-D model of a complex between an extracellular domain of a FcεRIα protein and a Fc-Cε3/Cε4 region that substantially represents the atomic coordinates specified (i.e., listed) in Table 1.

Table 1. Atomic coordinates of com14i_deposit.pdb

ATOM #	ATOM TYPE	RES	CHN	#	X	Y	Z	OCC	B
1	CB	VAL	A	1	-3.308	77.955	157.480	1.00	154.19
2	CG1	VAL	A	1	-2.631	78.371	156.184	1.00	159.57
3	CG2	VAL	A	1	-3.131	76.460	157.704	1.00	132.31
4	C	VAL	A	1	-2.948	80.258	158.492	1.00	178.97
5	O	VAL	A	1	-2.487	80.838	157.504	1.00	201.24
6	N	VAL	A	1	-3.255	78.193	159.967	1.00	154.76
7	CA	VAL	A	1	-2.715	78.740	158.688	1.00	168.39
8	N	PRO	A	2	-3.652	80.926	159.432	1.00	162.09
9	CD	PRO	A	2	-4.400	80.420	160.599	1.00	80.92
10	CA	PRO	A	2	-3.883	82.370	159.264	1.00	154.66
11	CB	PRO	A	2	-5.040	82.635	160.223	1.00	150.00
12	CG	PRO	A	2	-4.741	81.687	161.341	1.00	74.00
13	C	PRO	A	2	-2.659	83.238	159.588	1.00	157.76
14	O	PRO	A	2	-1.561	82.723	159.805	1.00	153.79
15	N	GLN	A	3	-2.850	84.557	159.604	1.00	167.42
16	CA	GLN	A	3	-1.767	85.480	159.940	1.00	118.16
17	CB	GLN	A	3	-2.084	86.902	159.460	1.00	89.25
18	CG	GLN	A	3	-1.705	87.173	158.009	1.00	165.02
19	CD	GLN	A	3	-2.117	88.561	157.535	1.00	182.69
20	OE1	GLN	A	3	-1.725	89.570	158.120	1.00	146.97
21	NE2	GLN	A	3	-2.908	88.616	156.462	1.00	178.25
22	C	GLN	A	3	-1.604	85.479	161.457	1.00	111.63
23	O	GLN	A	3	-2.582	85.634	162.192	1.00	63.56
24	N	LYS	A	4	-0.370	85.284	161.916	1.00	119.89
25	CA	LYS	A	4	-0.062	85.264	163.344	1.00	60.75
26	CB	LYS	A	4	1.263	84.535	163.607	1.00	99.96
27	CG	LYS	A	4	1.320	83.103	163.084	1.00	192.75
28	CD	LYS	A	4	2.645	82.417	163.434	1.00	187.23
29	CE	LYS	A	4	2.670	80.974	162.925	1.00	187.05
30	NZ	LYS	A	4	3.932	80.256	163.268	1.00	160.49
31	C	LYS	A	4	0.069	86.705	163.805	1.00	68.75
32	O	LYS	A	4	0.179	87.615	162.990	1.00	95.41
33	N	PRO	A	5	0.051	86.938	165.121	1.00	28.76
34	CD	PRO	A	5	-0.398	86.034	166.189	1.00	61.76
35	CA	PRO	A	5	0.176	88.304	165.632	1.00	48.28
36	CB	PRO	A	5	-0.576	88.231	166.949	1.00	43.06
37	CG	PRO	A	5	-0.226	86.882	167.417	1.00	11.05
38	C	PRO	A	5	1.638	88.734	165.804	1.00	63.30
39	O	PRO	A	5	2.469	87.967	166.293	1.00	54.45
40	N	LYS	A	6	1.944	89.961	165.388	1.00	63.56
41	CA	LYS	A	6	3.304	90.497	165.470	1.00	95.51
42	CB	LYS	A	6	3.647	91.212	164.151	1.00	110.28
43	CG	LYS	A	6	5.083	91.745	164.040	1.00	190.76
44	CD	LYS	A	6	6.120	90.634	163.856	1.00	206.32
45	CE	LYS	A	6	7.533	91.195	163.662	1.00	184.83
46	NZ	LYS	A	6	7.695	91.956	162.385	1.00	173.73
47	C	LYS	A	6	3.467	91.461	166.658	1.00	86.34
48	O	LYS	A	6	2.486	92.000	167.156	1.00	52.28
49	N	VAL	A	7	4.706	91.655	167.118	1.00	90.20
50	CA	VAL	A	7	5.010	92.561	168.234	1.00	22.49
51	CB	VAL	A	7	5.718	91.859	169.380	1.00	13.79
52	CG1	VAL	A	7	4.920	92.017	170.651	1.00	31.43

	53	CG2	VAL	A	7	5.937	90.401	169.033	1.00	92.97
	54	C	VAL	A	7	5.970	93.614	167.743	1.00	46.84
	55	O	VAL	A	7	6.960	93.293	167.084	1.00	64.82
	56	N	SER	A	8	5.680	94.867	168.065	1.00	36.46
	57	CA	SER	A	8	6.527	95.968	167.652	1.00	64.14
	58	CB	SER	A	8	5.721	96.962	166.816	1.00	31.16
	59	OG	SER	A	8	4.731	97.609	167.600	1.00	112.57
	60	C	SER	A	8	7.100	96.651	168.898	1.00	70.84
	61	O	SER	A	8	6.467	96.688	169.957	1.00	65.38
	62	N	LEU	A	9	8.311	97.173	168.772	1.00	34.20
	63	CA	LEU	A	9	8.962	97.844	169.877	1.00	17.68
	64	CB	LEU	A	9	10.335	97.254	170.082	1.00	35.73
	65	CG	LEU	A	9	10.470	95.929	170.799	1.00	5.42
	66	CD1	LEU	A	9	11.720	95.218	170.359	1.00	46.16
	67	CD2	LEU	A	9	10.552	96.200	172.244	1.00	38.43
	68	C	LEU	A	9	9.127	99.312	169.564	1.00	46.19
	69	O	LEU	A	9	9.420	99.680	168.438	1.00	59.24
	70	N	ASN	A	10	8.948	100.161	170.558	1.00	40.05
	71	CA	ASN	A	10	9.130	101.576	170.325	1.00	38.01
	72	CB	ASN	A	10	7.815	102.221	169.923	1.00	60.50
	73	CG	ASN	A	10	7.972	103.675	169.566	1.00	65.72
	74	OD1	ASN	A	10	7.555	104.551	170.319	1.00	78.78
	75	ND2	ASN	A	10	8.588	103.946	168.419	1.00	85.11
	76	C	ASN	A	10	9.683	102.237	171.567	1.00	46.63
	77	O	ASN	A	10	8.989	102.372	172.570	1.00	38.10
	78	N	PRO	A	11	10.952	102.661	171.513	1.00	36.23
	79	CD	PRO	A	11	11.474	103.662	172.446	1.00	18.87
	80	CA	PRO	A	11	11.852	102.543	170.367	1.00	23.13
	81	CB	PRO	A	11	12.980	103.476	170.747	1.00	49.98
	82	CG	PRO	A	11	12.266	104.514	171.534	1.00	45.32
	83	C	PRO	A	11	12.331	101.123	170.053	1.00	52.44
	84	O	PRO	A	11	12.575	100.322	170.964	1.00	41.38
	85	N	PRO	A	12	12.530	100.832	168.752	1.00	25.66
	86	CD	PRO	A	12	12.912	101.992	167.931	1.00	5.42
	87	CA	PRO	A	12	12.961	99.600	168.075	1.00	20.64
	88	CB	PRO	A	12	13.691	100.118	166.845	1.00	15.38
	89	CG	PRO	A	12	13.032	101.395	166.573	1.00	36.22
	90	C	PRO	A	12	13.858	98.688	168.875	1.00	26.86
	91	O	PRO	A	12	13.653	97.480	168.946	1.00	75.83
	92	N	TRP	A	13	14.881	99.297	169.445	1.00	51.05
	93	CA	TRP	A	13	15.898	98.623	170.226	1.00	46.59
	94	CB	TRP	A	13	16.675	99.690	170.966	1.00	5.42
	95	CG	TRP	A	13	16.638	100.993	170.234	1.00	17.98
	96	CD2	TRP	A	13	16.993	101.221	168.870	1.00	11.54
	97	CE2	TRP	A	13	16.869	102.602	168.631	1.00	36.13
	98	CE3	TRP	A	13	17.413	100.392	167.826	1.00	16.34
	99	CD1	TRP	A	13	16.310	102.211	170.749	1.00	79.53
	100	NE1	TRP	A	13	16.446	103.183	169.797	1.00	12.94
	101	CZ2	TRP	A	13	17.158	103.178	167.391	1.00	5.42
	102	CZ3	TRP	A	13	17.698	100.965	166.596	1.00	58.81
	103	CH2	TRP	A	13	17.572	102.346	166.393	1.00	14.55
	104	C	TRP	A	13	15.357	97.588	171.200	1.00	53.67
	105	O	TRP	A	13	14.615	97.929	172.116	1.00	40.75
	106	N	ASN	A	14	15.726	96.326	171.003	1.00	40.23
	107	CA	ASN	A	14	15.272	95.289	171.905	1.00	39.68

	108	CB	ASN	A	14	14.910	94.012	171.148	1.00	55.19
	109	CG	ASN	A	14	15.994	93.556	170.225	1.00	52.50
	110	OD1	ASN	A	14	17.116	93.309	170.653	1.00	34.32
	111	ND2	ASN	A	14	15.668	93.437	168.940	1.00	84.53
5	112	C	ASN	A	14	16.328	95.017	172.956	1.00	39.79
	113	O	ASN	A	14	16.232	94.049	173.704	1.00	68.24
	114	N	ARG	A	15	17.344	95.876	172.992	1.00	42.06
	115	CA	ARG	A	15	18.420	95.815	173.989	1.00	51.52
	116	CB	ARG	A	15	19.738	95.306	173.392	1.00	16.41
10	117	CG	ARG	A	15	20.077	95.790	172.006	1.00	43.90
	118	CD	ARG	A	15	21.494	95.348	171.646	1.00	69.87
	119	NE	ARG	A	15	21.733	93.931	171.916	1.00	49.77
	120	CZ	ARG	A	15	22.922	93.426	172.230	1.00	53.72
	121	NH1	ARG	A	15	23.985	94.212	172.321	1.00	38.62
15	122	NH2	ARG	A	15	23.050	92.129	172.455	1.00	109.67
	123	C	ARG	A	15	18.581	97.235	174.499	1.00	19.10
	124	O	ARG	A	15	18.822	98.147	173.725	1.00	10.96
	125	N	ILE	A	16	18.440	97.420	175.802	1.00	22.57
	126	CA	ILE	A	16	18.502	98.752	176.385	1.00	22.94
20	127	CB	ILE	A	16	17.101	99.298	176.601	1.00	32.81
	128	CG2	ILE	A	16	16.463	99.668	175.286	1.00	35.27
	129	CG1	ILE	A	16	16.283	98.250	177.349	1.00	10.08
	130	CD1	ILE	A	16	14.931	98.711	177.716	1.00	45.93
	131	C	ILE	A	16	19.170	98.826	177.745	1.00	47.61
25	132	O	ILE	A	16	19.175	97.854	178.495	1.00	52.58
	133	N	PHE	A	17	19.693	100.003	178.070	1.00	19.08
	134	CA	PHE	A	17	20.332	100.224	179.361	1.00	30.02
	135	CB	PHE	A	17	20.977	101.603	179.405	1.00	34.47
	136	CG	PHE	A	17	22.216	101.709	178.604	1.00	34.70
30	137	CD1	PHE	A	17	22.493	102.868	177.889	1.00	48.32
	138	CD2	PHE	A	17	23.105	100.649	178.544	1.00	11.47
	139	CE1	PHE	A	17	23.633	102.972	177.121	1.00	16.41
	140	CE2	PHE	A	17	24.246	100.739	177.782	1.00	40.21
	141	CZ	PHE	A	17	24.513	101.904	177.065	1.00	105.94
35	142	C	PHE	A	17	19.282	100.153	180.456	1.00	37.78
	143	O	PHE	A	17	18.146	100.564	180.256	1.00	17.05
	144	N	LYS	A	18	19.661	99.662	181.624	1.00	5.42
	145	CA	LYS	A	18	18.702	99.583	182.696	1.00	38.72
	146	CB	LYS	A	18	19.318	98.921	183.931	1.00	15.58
40	147	CG	LYS	A	18	19.768	99.862	185.000	1.00	22.71
	148	CD	LYS	A	18	20.290	99.109	186.226	1.00	39.40
	149	CE	LYS	A	18	19.181	98.710	187.181	1.00	57.95
	150	NZ	LYS	A	18	19.692	98.586	188.585	1.00	58.03
	151	C	LYS	A	18	18.213	100.972	183.034	1.00	9.14
45	152	O	LYS	A	18	18.976	101.919	183.006	1.00	14.56
	153	N	GLY	A	19	16.928	101.071	183.353	1.00	48.65
	154	CA	GLY	A	19	16.338	102.342	183.702	1.00	37.66
	155	C	GLY	A	19	15.760	103.020	182.487	1.00	11.50
	156	O	GLY	A	19	15.196	104.106	182.580	1.00	82.09
50	157	N	GLU	A	20	15.916	102.389	181.332	1.00	51.25
	158	CA	GLU	A	20	15.390	102.959	180.101	1.00	39.98
	159	CB	GLU	A	20	16.245	102.547	178.901	1.00	61.38
	160	CG	GLU	A	20	17.645	103.141	178.937	1.00	107.42
	161	CD	GLU	A	20	18.374	103.073	177.608	1.00	75.17
55	162	OE1	GLU	A	20	19.490	103.620	177.537	1.00	70.97

	163	OE2	GLU	A	20	17.847	102.483	176.639	1.00	72.76
	164	C	GLU	A	20	13.950	102.532	179.893	1.00	47.68
	165	O	GLU	A	20	13.449	101.624	180.565	1.00	16.47
	166	N	ASN	A	21	13.280	103.200	178.964	1.00	51.83
5	167	CA	ASN	A	21	11.885	102.910	178.692	1.00	39.65
	168	CB	ASN	A	21	11.057	104.195	178.786	1.00	36.44
	169	CG	ASN	A	21	11.008	104.762	180.191	1.00	24.19
	170	OD1	ASN	A	21	10.954	104.009	181.164	1.00	25.70
	171	ND2	ASN	A	21	11.002	106.089	180.298	1.00	72.05
10	172	C	ASN	A	21	11.653	102.271	177.340	1.00	14.38
	173	O	ASN	A	21	12.362	102.554	176.384	1.00	96.93
	174	N	VAL	A	22	10.651	101.405	177.270	1.00	55.87
	175	CA	VAL	A	22	10.305	100.748	176.023	1.00	39.97
	176	CB	VAL	A	22	11.168	99.525	175.769	1.00	23.77
15	177	CG1	VAL	A	22	10.880	98.461	176.789	1.00	24.69
	178	CG2	VAL	A	22	10.896	99.013	174.395	1.00	10.67
	179	C	VAL	A	22	8.861	100.308	176.057	1.00	39.52
	180	O	VAL	A	22	8.299	100.143	177.134	1.00	50.04
	181	N	THR	A	23	8.273	100.106	174.879	1.00	35.08
20	182	CA	THR	A	23	6.876	99.689	174.758	1.00	50.38
	183	CB	THR	A	23	5.982	100.883	174.356	1.00	15.46
	184	OG1	THR	A	23	5.325	101.397	175.515	1.00	51.09
	185	CG2	THR	A	23	4.944	100.470	173.342	1.00	53.00
	186	C	THR	A	23	6.638	98.564	173.758	1.00	24.12
25	187	O	THR	A	23	7.121	98.601	172.629	1.00	33.75
	188	N	LEU	A	24	5.869	97.567	174.170	1.00	32.66
	189	CA	LEU	A	24	5.565	96.463	173.278	1.00	45.63
	190	CB	LEU	A	24	5.754	95.119	173.987	1.00	23.83
	191	CG	LEU	A	24	7.072	94.939	174.739	1.00	28.78
30	192	CD1	LEU	A	24	7.381	93.488	174.933	1.00	19.89
	193	CD2	LEU	A	24	8.159	95.572	173.969	1.00	5.42
	194	C	LEU	A	24	4.128	96.607	172.822	1.00	44.86
	195	O	LEU	A	24	3.248	96.866	173.635	1.00	52.63
	196	N	THR	A	25	3.895	96.444	171.523	1.00	52.39
35	197	CA	THR	A	25	2.554	96.550	170.965	1.00	46.08
	198	CB	THR	A	25	2.454	97.761	170.049	1.00	24.50
	199	OG1	THR	A	25	3.088	98.884	170.673	1.00	62.13
	200	CG2	THR	A	25	1.016	98.098	169.807	1.00	77.17
	201	C	THR	A	25	2.233	95.282	170.174	1.00	59.55
40	202	O	THR	A	25	3.120	94.707	169.542	1.00	36.44
	203	N	CYS	A	26	0.970	94.852	170.215	1.00	59.40
	204	CA	CYS	A	26	0.520	93.642	169.525	1.00	38.53
	205	C	CYS	A	26	-0.343	94.009	168.318	1.00	42.63
	206	O	CYS	A	26	-1.322	94.734	168.447	1.00	77.67
45	207	CB	CYS	A	26	-0.256	92.757	170.514	1.00	31.91
	208	SG	CYS	A	26	-0.296	90.939	170.208	1.00	112.14
	209	N	ASN	A	27	0.083	93.514	167.154	1.00	114.86
	210	CA	ASN	A	27	-0.506	93.677	165.805	1.00	124.26
	211	CB	ASN	A	27	-0.765	92.286	165.217	1.00	138.85
50	212	CG	ASN	A	27	-0.588	92.249	163.708	1.00	187.97
	213	OD1	ASN	A	27	-0.071	93.196	163.106	1.00	180.59
	214	ND2	ASN	A	27	-0.999	91.145	163.090	1.00	211.12
	215	C	ASN	A	27	-1.717	94.563	165.469	1.00	69.87
	216	O	ASN	A	27	-2.604	94.788	166.278	1.00	99.87
55	217	N	GLY	A	28	-1.737	95.043	164.228	1.00	93.93

	218	CA	GLY	A	28	-2.818	95.887	163.752	1.00	33.38
	219	C	GLY	A	28	-3.811	95.070	162.949	1.00	71.27
	220	O	GLY	A	28	-4.658	95.611	162.243	1.00	61.63
	221	N	ASN	A	29	-3.686	93.752	163.064	1.00	116.52
5	222	CA	ASN	A	29	-4.550	92.783	162.388	1.00	70.71
	223	CB	ASN	A	29	-3.729	91.533	162.062	1.00	121.95
	224	CG	ASN	A	29	-4.164	90.852	160.783	1.00	150.49
	225	OD1	ASN	A	29	-4.247	91.480	159.727	1.00	172.84
	226	ND2	ASN	A	29	-4.428	89.550	160.868	1.00	174.68
10	227	C	ASN	A	29	-5.658	92.466	163.405	1.00	97.53
	228	O	ASN	A	29	-6.252	91.389	163.421	1.00	106.16
	229	N	ASN	A	30	-5.886	93.448	164.265	1.00	53.59
	230	CA	ASN	A	30	-6.878	93.432	165.332	1.00	80.30
	231	CB	ASN	A	30	-6.317	92.689	166.558	1.00	85.88
15	232	CG	ASN	A	30	-7.040	93.041	167.875	1.00	109.70
	233	OD1	ASN	A	30	-8.256	92.883	168.011	1.00	70.68
	234	ND2	ASN	A	30	-6.272	93.507	168.851	1.00	35.68
	235	C	ASN	A	30	-7.041	94.917	165.623	1.00	78.22
	236	O	ASN	A	30	-6.772	95.363	166.729	1.00	51.75
20	237	N	PHE	A	31	-7.493	95.667	164.617	1.00	89.72
	238	CA	PHE	A	31	-7.629	97.125	164.709	1.00	96.61
	239	CB	PHE	A	31	-7.900	97.716	163.320	1.00	115.42
	240	CG	PHE	A	31	-7.680	99.211	163.242	1.00	120.39
	241	CD1	PHE	A	31	-6.403	99.745	163.398	1.00	112.19
25	242	CD2	PHE	A	31	-8.746	100.083	163.023	1.00	119.97
	243	CE1	PHE	A	31	-6.190	101.121	163.339	1.00	72.84
	244	CE2	PHE	A	31	-8.544	101.460	162.962	1.00	60.99
	245	CZ	PHE	A	31	-7.262	101.978	163.122	1.00	105.12
	246	C	PHE	A	31	-8.585	97.783	165.707	1.00	94.85
30	247	O	PHE	A	31	-8.131	98.494	166.601	1.00	127.53
	248	N	PHE	A	32	-9.894	97.596	165.564	1.00	91.11
	249	CA	PHE	A	32	-10.818	98.248	166.500	1.00	92.26
	250	CB	PHE	A	32	-12.272	98.103	166.052	1.00	93.61
	251	CG	PHE	A	32	-12.504	98.467	164.625	1.00	103.12
35	252	CD1	PHE	A	32	-12.136	97.591	163.600	1.00	99.09
	253	CD2	PHE	A	32	-13.064	99.693	164.298	1.00	32.51
	254	CE1	PHE	A	32	-12.320	97.933	162.268	1.00	63.07
	255	CE2	PHE	A	32	-13.251	100.044	162.974	1.00	108.41
	256	CZ	PHE	A	32	-12.877	99.160	161.953	1.00	118.33
40	257	C	PHE	A	32	-10.673	97.618	167.867	1.00	102.23
	258	O	PHE	A	32	-11.305	98.050	168.838	1.00	76.95
	259	N	GLU	A	33	-9.827	96.593	167.918	1.00	90.59
	260	CA	GLU	A	33	-9.567	95.837	169.127	1.00	58.80
	261	CB	GLU	A	33	-9.193	96.766	170.287	1.00	34.16
45	262	CG	GLU	A	33	-7.709	97.116	170.319	1.00	83.37
	263	CD	GLU	A	33	-7.302	97.846	171.583	1.00	138.46
	264	OE1	GLU	A	33	-7.822	97.498	172.666	1.00	156.92
	265	OE2	GLU	A	33	-6.450	98.757	171.494	1.00	143.48
	266	C	GLU	A	33	-10.807	95.038	169.458	1.00	51.35
50	267	O	GLU	A	33	-11.670	95.489	170.207	1.00	76.71
	268	N	VAL	A	34	-10.889	93.849	168.874	1.00	40.24
	269	CA	VAL	A	34	-12.018	92.963	169.092	1.00	63.51
	270	CB	VAL	A	34	-12.369	92.212	167.815	1.00	12.87
	271	CG1	VAL	A	34	-12.724	93.199	166.743	1.00	47.66
55	272	CG2	VAL	A	34	-11.194	91.350	167.382	1.00	80.18

	273	C	VAL	A	34	-11.691	91.960	170.185	1.00	48.93
	274	O	VAL	A	34	-12.584	91.300	170.719	1.00	66.41
	275	N	SER	A	35	-10.411	91.840	170.518	1.00	40.51
	276	CA	SER	A	35	-10.027	90.913	171.568	1.00	79.37
5	277	CB	SER	A	35	-9.460	89.642	170.974	1.00	33.93
	278	OG	SER	A	35	-8.107	89.851	170.650	1.00	44.80
	279	C	SER	A	35	-8.991	91.484	172.530	1.00	83.70
	280	O	SER	A	35	-8.097	92.242	172.139	1.00	52.41
	281	N	SER	A	36	-9.127	91.112	173.798	1.00	57.27
10	282	CA	SER	A	36	-8.195	91.539	174.819	1.00	23.32
	283	CB	SER	A	36	-8.600	90.956	176.156	1.00	119.43
	284	OG	SER	A	36	-8.593	89.547	176.089	1.00	43.01
	285	C	SER	A	36	-6.879	90.929	174.408	1.00	49.51
	286	O	SER	A	36	-6.857	89.930	173.702	1.00	34.96
15	287	N	THR	A	37	-5.780	91.517	174.854	1.00	52.38
	288	CA	THR	A	37	-4.466	90.996	174.516	1.00	34.52
	289	CB	THR	A	37	-3.501	92.113	174.181	1.00	28.99
	290	OG1	THR	A	37	-4.074	92.965	173.182	1.00	95.55
	291	CG2	THR	A	37	-2.211	91.537	173.682	1.00	68.24
20	292	C	THR	A	37	-3.890	90.283	175.710	1.00	57.63
	293	O	THR	A	37	-4.159	90.662	176.848	1.00	34.77
	294	N	LYS	A	38	-3.109	89.241	175.469	1.00	28.90
	295	CA	LYS	A	38	-2.491	88.551	176.588	1.00	65.81
	296	CB	LYS	A	38	-3.111	87.179	176.799	1.00	34.97
25	297	CG	LYS	A	38	-3.818	86.631	175.615	1.00	36.39
	298	CD	LYS	A	38	-5.098	85.965	176.076	1.00	85.18
	299	CE	LYS	A	38	-6.234	86.958	176.203	1.00	26.12
	300	NZ	LYS	A	38	-7.146	86.806	175.029	1.00	20.00
	301	C	LYS	A	38	-0.990	88.454	176.381	1.00	79.44
30	302	O	LYS	A	38	-0.523	87.805	175.444	1.00	44.12
	303	N	TRP	A	39	-0.256	89.130	177.268	1.00	74.45
	304	CA	TRP	A	39	1.198	89.204	177.230	1.00	12.82
	305	CB	TRP	A	39	1.656	90.574	177.704	1.00	55.75
	306	CG	TRP	A	39	1.180	91.696	176.875	1.00	17.73
35	307	CD2	TRP	A	39	1.763	92.144	175.661	1.00	20.84
	308	CE2	TRP	A	39	0.957	93.195	175.175	1.00	24.82
	309	CE3	TRP	A	39	2.889	91.757	174.930	1.00	15.24
	310	CD1	TRP	A	39	0.069	92.473	177.082	1.00	45.58
	311	NE1	TRP	A	39	-0.072	93.374	176.060	1.00	18.25
40	312	CZ2	TRP	A	39	1.247	93.864	173.990	1.00	26.70
	313	CZ3	TRP	A	39	3.177	92.419	173.751	1.00	13.49
	314	CH2	TRP	A	39	2.360	93.463	173.293	1.00	70.81
	315	C	TRP	A	39	1.847	88.166	178.109	1.00	55.49
	316	O	TRP	A	39	1.417	87.945	179.236	1.00	33.26
45	317	N	PHE	A	40	2.916	87.566	177.604	1.00	28.08
	318	CA	PHE	A	40	3.640	86.538	178.331	1.00	19.83
	319	CB	PHE	A	40	3.527	85.229	177.574	1.00	69.82
	320	CG	PHE	A	40	2.137	84.682	177.528	1.00	65.09
	321	CD1	PHE	A	40	1.608	84.205	176.338	1.00	50.58
50	322	CD2	PHE	A	40	1.367	84.614	178.680	1.00	53.63
	323	CE1	PHE	A	40	0.341	83.673	176.300	1.00	68.98
	324	CE2	PHE	A	40	0.105	84.083	178.646	1.00	26.70
	325	CZ	PHE	A	40	-0.414	83.611	177.459	1.00	85.38
	326	C	PHE	A	40	5.112	86.889	178.522	1.00	83.34
55	327	O	PHE	A	40	5.835	87.108	177.546	1.00	65.61

	328	N	HIS	A	41	5.549	86.924	179.780	1.00	49.52
	329	CA	HIS	A	41	6.929	87.243	180.121	1.00	41.84
	330	CB	HIS	A	41	6.950	88.359	181.166	1.00	82.94
	331	CG	HIS	A	41	8.325	88.832	181.529	1.00	109.26
5	332	CD2	HIS	A	41	8.822	89.302	182.698	1.00	54.39
	333	ND1	HIS	A	41	9.361	88.901	180.618	1.00	50.58
	334	CE1	HIS	A	41	10.433	89.389	181.213	1.00	51.90
	335	NE2	HIS	A	41	10.133	89.642	182.475	1.00	80.09
	336	C	HIS	A	41	7.671	86.006	180.630	1.00	66.77
10	337	O	HIS	A	41	7.413	85.511	181.729	1.00	49.22
	338	N	ASN	A	42	8.594	85.513	179.806	1.00	91.49
	339	CA	ASN	A	42	9.383	84.329	180.122	1.00	83.79
	340	CB	ASN	A	42	10.313	84.601	181.315	1.00	71.40
	341	CG	ASN	A	42	11.573	85.360	180.915	1.00	72.11
15	342	OD1	ASN	A	42	11.498	86.390	180.243	1.00	85.40
	343	ND2	ASN	A	42	12.732	84.857	181.333	1.00	104.80
	344	C	ASN	A	42	8.464	83.156	180.421	1.00	77.24
	345	O	ASN	A	42	8.923	82.037	180.657	1.00	110.53
	346	N	GLY	A	43	7.162	83.418	180.389	1.00	47.35
20	347	CA	GLY	A	43	6.201	82.378	180.662	1.00	34.83
	348	C	GLY	A	43	4.909	82.844	181.300	1.00	49.78
	349	O	GLY	A	43	3.855	82.683	180.707	1.00	48.66
	350	N	SER	A	44	4.971	83.412	182.499	1.00	38.80
	351	CA	SER	A	44	3.760	83.860	183.181	1.00	51.26
25	352	CB	SER	A	44	4.090	84.455	184.553	1.00	115.68
	353	OG	SER	A	44	4.024	83.466	185.572	1.00	158.60
	354	C	SER	A	44	2.933	84.859	182.407	1.00	57.42
	355	O	SER	A	44	3.443	85.594	181.569	1.00	48.28
	356	N	LEU	A	45	1.639	84.871	182.708	1.00	78.92
30	357	CA	LEU	A	45	0.698	85.769	182.062	1.00	43.70
	358	CB	LEU	A	45	-0.728	85.215	182.177	1.00	33.26
	359	CG	LEU	A	45	-1.810	86.048	181.475	1.00	38.67
	360	CD1	LEU	A	45	-1.934	85.532	180.084	1.00	20.12
	361	CD2	LEU	A	45	-3.171	85.962	182.155	1.00	16.35
35	362	C	LEU	A	45	0.755	87.134	182.731	1.00	45.32
	363	O	LEU	A	45	0.531	87.243	183.928	1.00	46.93
	364	N	SER	A	46	1.053	88.176	181.964	1.00	43.39
	365	CA	SER	A	46	1.100	89.513	182.530	1.00	61.73
	366	CB	SER	A	46	1.808	90.469	181.584	1.00	36.13
40	367	OG	SER	A	46	1.827	91.769	182.137	1.00	89.66
	368	C	SER	A	46	-0.316	90.006	182.778	1.00	33.11
	369	O	SER	A	46	-1.245	89.564	182.105	1.00	74.17
	370	N	GLU	A	47	-0.475	90.927	183.727	1.00	51.16
	371	CA	GLU	A	47	-1.794	91.467	184.059	1.00	59.94
45	372	CB	GLU	A	47	-1.876	91.906	185.536	1.00	102.95
	373	CG	GLU	A	47	-1.109	93.176	185.915	1.00	167.20
	374	CD	GLU	A	47	-1.380	93.622	187.356	1.00	181.03
	375	OE1	GLU	A	47	-2.558	93.869	187.696	1.00	179.85
	376	OE2	GLU	A	47	-0.420	93.729	188.151	1.00	185.11
50	377	C	GLU	A	47	-2.257	92.613	183.169	1.00	72.12
	378	O	GLU	A	47	-3.330	93.173	183.399	1.00	64.78
	379	N	GLU	A	48	-1.459	92.977	182.168	1.00	30.89
	380	CA	GLU	A	48	-1.875	94.033	181.255	1.00	56.44
	381	CB	GLU	A	48	-0.689	94.737	180.606	1.00	83.36
55	382	CG	GLU	A	48	-1.099	95.797	179.581	1.00	51.54

	383	CD	GLU	A	48	-1.832	96.978	180.201	1.00	104.67
	384	OE1	GLU	A	48	-2.168	96.919	181.403	1.00	138.97
	385	OE2	GLU	A	48	-2.077	97.968	179.481	1.00	142.55
	386	C	GLU	A	48	-2.664	93.332	180.178	1.00	67.47
5	387	O	GLU	A	48	-2.224	92.303	179.658	1.00	72.45
	388	N	THR	A	49	-3.827	93.874	179.841	1.00	44.94
	389	CA	THR	A	49	-4.650	93.249	178.824	1.00	53.65
	390	CB	THR	A	49	-6.057	92.937	179.361	1.00	38.32
	391	OG1	THR	A	49	-6.717	94.152	179.731	1.00	71.69
10	392	CG2	THR	A	49	-5.957	92.031	180.574	1.00	68.17
	393	C	THR	A	49	-4.773	94.090	177.570	1.00	42.57
	394	O	THR	A	49	-5.323	93.620	176.572	1.00	55.30
	395	N	ASN	A	50	-4.244	95.316	177.618	1.00	39.30
	396	CA	ASN	A	50	-4.308	96.238	176.481	1.00	35.89
15	397	CB	ASN	A	50	-4.131	97.680	176.959	1.00	40.10
	398	CG	ASN	A	50	-5.248	98.123	177.888	1.00	104.98
	399	OD1	ASN	A	50	-6.425	97.966	177.566	1.00	104.75
	400	ND2	ASN	A	50	-4.888	98.684	179.044	1.00	117.05
	401	C	ASN	A	50	-3.331	95.925	175.343	1.00	40.37
20	402	O	ASN	A	50	-2.419	95.117	175.484	1.00	38.49
	403	N	SER	A	51	-3.545	96.576	174.208	1.00	50.20
	404	CA	SER	A	51	-2.751	96.358	173.012	1.00	23.03
	405	CB	SER	A	51	-3.377	97.148	171.867	1.00	91.07
	406	OG	SER	A	51	-2.997	96.611	170.612	1.00	171.49
25	407	C	SER	A	51	-1.259	96.682	173.121	1.00	69.60
	408	O	SER	A	51	-0.437	96.164	172.360	1.00	46.29
	409	N	SER	A	52	-0.896	97.547	174.055	1.00	45.59
	410	CA	SER	A	52	0.504	97.893	174.211	1.00	54.59
	411	CB	SER	A	52	0.768	99.315	173.715	1.00	8.18
30	412	OG	SER	A	52	-0.152	100.219	174.304	1.00	136.82
	413	C	SER	A	52	0.905	97.753	175.661	1.00	27.90
	414	O	SER	A	52	0.190	98.183	176.556	1.00	44.58
	415	N	LEU	A	53	2.053	97.118	175.870	1.00	63.94
	416	CA	LEU	A	53	2.613	96.882	177.188	1.00	46.87
35	417	CB	LEU	A	53	3.060	95.430	177.306	1.00	46.27
	418	CG	LEU	A	53	3.830	95.066	178.569	1.00	30.42
	419	CD1	LEU	A	53	2.999	95.372	179.782	1.00	91.21
	420	CD2	LEU	A	53	4.172	93.618	178.534	1.00	12.37
	421	C	LEU	A	53	3.811	97.789	177.394	1.00	56.10
40	422	O	LEU	A	53	4.693	97.864	176.539	1.00	60.76
	423	N	ASN	A	54	3.841	98.474	178.529	1.00	47.36
	424	CA	ASN	A	54	4.937	99.378	178.841	1.00	46.29
	425	CB	ASN	A	54	4.403	100.640	179.506	1.00	42.78
	426	CG	ASN	A	54	3.436	101.383	178.631	1.00	41.09
45	427	OD1	ASN	A	54	3.786	101.807	177.538	1.00	49.17
	428	ND2	ASN	A	54	2.207	101.545	179.104	1.00	84.48
	429	C	ASN	A	54	5.976	98.749	179.753	1.00	33.11
	430	O	ASN	A	54	5.771	97.691	180.331	1.00	62.93
	431	N	ILE	A	55	7.106	99.422	179.867	1.00	61.10
50	432	CA	ILE	A	55	8.189	98.981	180.719	1.00	47.90
	433	CB	ILE	A	55	9.217	98.157	179.946	1.00	13.22
	434	CG2	ILE	A	55	10.449	97.922	180.795	1.00	78.62
	435	CG1	ILE	A	55	8.619	96.807	179.586	1.00	27.07
	436	CD1	ILE	A	55	9.649	95.826	179.074	1.00	30.03
55	437	C	ILE	A	55	8.829	100.267	181.189	1.00	83.99

	438	O	ILE	A	55	9.222	101.101	180.371	1.00	75.43
	439	N	VAL	A	56	8.923	100.443	182.501	1.00	33.41
	440	CA	VAL	A	56	9.505	101.660	183.024	1.00	49.06
	441	CB	VAL	A	56	8.444	102.453	183.758	1.00	15.18
5	442	CG1	VAL	A	56	9.046	103.714	184.329	1.00	108.22
	443	CG2	VAL	A	56	7.328	102.792	182.789	1.00	29.46
	444	C	VAL	A	56	10.706	101.421	183.923	1.00	69.57
	445	O	VAL	A	56	10.757	100.422	184.648	1.00	49.84
	446	N	ASN	A	57	11.664	102.348	183.872	1.00	28.08
10	447	CA	ASN	A	57	12.887	102.233	184.656	1.00	76.91
	448	CB	ASN	A	57	12.673	102.732	186.090	1.00	41.01
	449	CG	ASN	A	57	12.080	104.137	186.133	1.00	126.97
	450	OD1	ASN	A	57	12.275	104.939	185.212	1.00	85.74
	451	ND2	ASN	A	57	11.359	104.444	187.211	1.00	113.52
15	452	C	ASN	A	57	13.219	100.756	184.636	1.00	51.64
	453	O	ASN	A	57	13.382	100.110	185.669	1.00	51.28
	454	N	ALA	A	58	13.294	100.237	183.419	1.00	5.42
	455	CA	ALA	A	58	13.562	98.838	183.185	1.00	28.33
	456	CB	ALA	A	58	13.971	98.636	181.763	1.00	26.01
20	457	C	ALA	A	58	14.604	98.236	184.083	1.00	26.51
	458	O	ALA	A	58	15.769	98.571	183.983	1.00	45.62
	459	N	LYS	A	59	14.182	97.336	184.962	1.00	54.38
	460	CA	LYS	A	59	15.114	96.654	185.838	1.00	54.01
	461	CB	LYS	A	59	14.388	96.159	187.080	1.00	49.09
25	462	CG	LYS	A	59	15.301	95.437	188.061	1.00	140.01
	463	CD	LYS	A	59	16.432	96.316	188.603	1.00	80.75
	464	CE	LYS	A	59	17.313	95.516	189.541	1.00	71.72
	465	NZ	LYS	A	59	17.864	94.316	188.836	1.00	63.79
	466	C	LYS	A	59	15.681	95.481	185.031	1.00	38.80
30	467	O	LYS	A	59	15.234	95.229	183.920	1.00	40.61
	468	N	PHE	A	60	16.673	94.771	185.549	1.00	36.75
	469	CA	PHE	A	60	17.207	93.658	184.776	1.00	26.24
	470	CB	PHE	A	60	18.416	93.052	185.445	1.00	43.58
	471	CG	PHE	A	60	19.579	93.957	185.491	1.00	76.01
35	472	CD1	PHE	A	60	19.616	95.002	186.399	1.00	61.74
	473	CD2	PHE	A	60	20.634	93.787	184.606	1.00	45.10
	474	CE1	PHE	A	60	20.691	95.867	186.419	1.00	50.78
	475	CE2	PHE	A	60	21.712	94.651	184.621	1.00	21.53
	476	CZ	PHE	A	60	21.741	95.689	185.525	1.00	37.49
40	477	C	PHE	A	60	16.169	92.580	184.653	1.00	69.55
	478	O	PHE	A	60	16.062	91.924	183.617	1.00	29.04
	479	N	GLU	A	61	15.429	92.395	185.742	1.00	35.52
	480	CA	GLU	A	61	14.371	91.406	185.823	1.00	48.73
	481	CB	GLU	A	61	13.552	91.627	187.104	1.00	104.40
45	482	CG	GLU	A	61	14.214	91.078	188.378	1.00	176.16
	483	CD	GLU	A	61	15.427	91.882	188.853	1.00	198.10
	484	OE1	GLU	A	61	15.236	93.016	189.341	1.00	190.74
	485	OE2	GLU	A	61	16.573	91.381	188.747	1.00	185.84
	486	C	GLU	A	61	13.468	91.481	184.602	1.00	72.09
50	487	O	GLU	A	61	12.846	90.496	184.214	1.00	44.44
	488	N	ASP	A	62	13.418	92.657	183.987	1.00	43.54
	489	CA	ASP	A	62	12.589	92.874	182.816	1.00	19.32
	490	CB	ASP	A	62	12.312	94.371	182.659	1.00	5.54
	491	CG	ASP	A	62	11.524	94.956	183.850	1.00	95.59
55	492	OD1	ASP	A	62	10.790	94.200	184.540	1.00	64.35

	493	OD2	ASP	A	62	11.618	96.182	184.091	1.00	64.15
	494	C	ASP	A	62	13.156	92.283	181.519	1.00	28.80
	495	O	ASP	A	62	12.492	92.276	180.483	1.00	23.08
	496	N	SER	A	63	14.378	91.772	181.558	1.00	39.71
5	497	CA	SER	A	63	14.940	91.174	180.353	1.00	51.88
	498	CB	SER	A	63	16.395	90.770	180.579	1.00	43.74
	499	OG	SER	A	63	17.214	91.898	180.813	1.00	80.04
	500	C	SER	A	63	14.108	89.938	180.092	1.00	33.07
	501	O	SER	A	63	13.290	89.573	180.919	1.00	42.64
10	502	N	GLY	A	64	14.295	89.293	178.949	1.00	33.31
	503	CA	GLY	A	64	13.529	88.085	178.701	1.00	47.82
	504	C	GLY	A	64	12.703	87.912	177.437	1.00	78.77
	505	O	GLY	A	64	12.738	88.718	176.503	1.00	41.30
	506	N	GLU	A	65	11.947	86.819	177.426	1.00	38.56
15	507	CA	GLU	A	65	11.096	86.471	176.303	1.00	61.82
	508	CB	GLU	A	65	11.022	84.950	176.157	1.00	56.45
	509	CG	GLU	A	65	9.864	84.452	175.314	1.00	60.09
	510	CD	GLU	A	65	9.860	82.944	175.145	1.00	97.74
	511	OE1	GLU	A	65	9.816	82.221	176.165	1.00	145.16
20	512	OE2	GLU	A	65	9.898	82.480	173.987	1.00	99.49
	513	C	GLU	A	65	9.693	87.030	176.447	1.00	47.26
	514	O	GLU	A	65	9.000	86.742	177.415	1.00	50.30
	515	N	TYR	A	66	9.282	87.829	175.468	1.00	55.07
	516	CA	TYR	A	66	7.951	88.414	175.462	1.00	29.51
25	517	CB	TYR	A	66	8.037	89.931	175.342	1.00	33.26
	518	CG	TYR	A	66	8.495	90.627	176.599	1.00	36.26
	519	CD1	TYR	A	66	9.844	90.671	176.946	1.00	54.70
	520	CE1	TYR	A	66	10.264	91.287	178.118	1.00	20.05
	521	CD2	TYR	A	66	7.574	91.217	177.456	1.00	14.39
30	522	CE2	TYR	A	66	7.978	91.827	178.623	1.00	52.79
	523	CZ	TYR	A	66	9.323	91.862	178.952	1.00	76.87
	524	OH	TYR	A	66	9.709	92.485	180.115	1.00	49.97
	525	C	TYR	A	66	7.135	87.859	174.296	1.00	58.69
	526	O	TYR	A	66	7.653	87.704	173.190	1.00	49.90
35	527	N	LYS	A	67	5.866	87.548	174.560	1.00	53.66
	528	CA	LYS	A	67	4.946	87.023	173.550	1.00	38.25
	529	CB	LYS	A	67	4.957	85.504	173.534	1.00	5.42
	530	CG	LYS	A	67	6.054	84.856	172.724	1.00	46.81
	531	CD	LYS	A	67	5.918	83.324	172.794	1.00	100.90
40	532	CE	LYS	A	67	5.849	82.829	174.249	1.00	91.92
	533	NZ	LYS	A	67	5.762	81.347	174.372	1.00	45.56
	534	C	LYS	A	67	3.530	87.460	173.867	1.00	67.55
	535	O	LYS	A	67	3.164	87.560	175.038	1.00	52.62
	536	N	CYS	A	68	2.741	87.730	172.830	1.00	27.93
45	537	CA	CYS	A	68	1.346	88.113	173.023	1.00	62.04
	538	C	CYS	A	68	0.522	87.234	172.111	1.00	74.23
	539	O	CYS	A	68	0.992	86.816	171.060	1.00	45.57
	540	CB	CYS	A	68	1.092	89.597	172.678	1.00	29.72
	541	SG	CYS	A	68	1.419	90.098	170.952	1.00	99.54
50	542	N	GLN	A	69	-0.695	86.920	172.525	1.00	33.27
	543	CA	GLN	A	69	-1.553	86.119	171.681	1.00	50.08
	544	CB	GLN	A	69	-1.489	84.636	172.081	1.00	48.05
	545	CG	GLN	A	69	-2.425	84.215	173.203	1.00	61.10
	546	CD	GLN	A	69	-2.526	82.705	173.318	1.00	71.23
55	547	OE1	GLN	A	69	-2.813	82.023	172.336	1.00	91.00

	548	NE2	GLN	A	69	-2.294	82.174	174.516	1.00	82.52
	549	C	GLN	A	69	-2.951	86.698	171.837	1.00	82.00
	550	O	GLN	A	69	-3.259	87.275	172.881	1.00	33.84
	551	N	HIS	A	70	-3.780	86.569	170.798	1.00	41.19
5	552	CA	HIS	A	70	-5.135	87.114	170.836	1.00	43.14
	553	CB	HIS	A	70	-5.503	87.695	169.484	1.00	74.38
	554	CG	HIS	A	70	-4.758	88.949	169.156	1.00	88.05
	555	CD2	HIS	A	70	-4.093	89.321	168.038	1.00	38.05
	556	ND1	HIS	A	70	-4.693	90.022	170.019	1.00	28.06
10	557	CE1	HIS	A	70	-4.025	91.004	169.442	1.00	56.78
	558	NE2	HIS	A	70	-3.651	90.603	168.240	1.00	58.51
	559	C	HIS	A	70	-6.193	86.125	171.279	1.00	67.91
	560	O	HIS	A	70	-6.224	85.738	172.448	1.00	57.73
	561	N	GLN	A	71	-7.103	85.741	170.393	1.00	57.13
15	562	CA	GLN	A	71	-8.074	84.755	170.836	1.00	92.00
	563	CB	GLN	A	71	-9.521	85.291	170.854	1.00	30.07
	564	CG	GLN	A	71	-9.993	86.007	169.632	1.00	41.74
	565	CD	GLN	A	71	-11.225	86.849	169.901	1.00	87.95
	566	OE1	GLN	A	71	-11.837	86.748	170.965	1.00	35.65
20	567	NE2	GLN	A	71	-11.597	87.690	168.927	1.00	53.82
	568	C	GLN	A	71	-7.944	83.483	170.037	1.00	34.54
	569	O	GLN	A	71	-8.800	82.610	170.102	1.00	84.17
	570	N	GLN	A	72	-6.840	83.376	169.302	1.00	51.65
	571	CA	GLN	A	72	-6.556	82.167	168.543	1.00	53.66
25	572	CB	GLN	A	72	-6.029	82.497	167.153	1.00	40.22
	573	CG	GLN	A	72	-7.084	82.254	166.099	1.00	83.83
	574	CD	GLN	A	72	-6.726	82.827	164.759	1.00	29.94
	575	OE1	GLN	A	72	-5.765	82.397	164.129	1.00	114.76
	576	NE2	GLN	A	72	-7.500	83.813	164.310	1.00	98.66
30	577	C	GLN	A	72	-5.573	81.267	169.288	1.00	43.67
	578	O	GLN	A	72	-5.373	81.404	170.490	1.00	58.65
	579	N	VAL	A	73	-4.958	80.337	168.583	1.00	56.83
	580	CA	VAL	A	73	-4.054	79.418	169.252	1.00	51.40
	581	CB	VAL	A	73	-4.188	77.998	168.669	1.00	106.92
35	582	CG1	VAL	A	73	-3.580	77.944	167.252	1.00	46.73
	583	CG2	VAL	A	73	-3.536	76.996	169.604	1.00	22.40
	584	C	VAL	A	73	-2.622	79.862	169.121	1.00	64.50
	585	O	VAL	A	73	-1.851	79.805	170.077	1.00	72.42
	586	N	ALA	A	74	-2.270	80.292	167.919	1.00	78.31
40	587	CA	ALA	A	74	-0.924	80.744	167.649	1.00	78.26
	588	CB	ALA	A	74	-0.740	80.981	166.166	1.00	125.54
	589	C	ALA	A	74	-0.649	82.019	168.418	1.00	66.03
	590	O	ALA	A	74	-1.553	82.817	168.681	1.00	85.24
	591	N	GLU	A	75	0.616	82.194	168.768	1.00	67.79
45	592	CA	GLU	A	75	1.082	83.347	169.516	1.00	53.61
	593	CB	GLU	A	75	1.465	82.908	170.935	1.00	18.85
	594	CG	GLU	A	75	2.031	81.485	170.991	1.00	113.19
	595	CD	GLU	A	75	2.349	81.011	172.398	1.00	127.80
	596	OE1	GLU	A	75	1.510	81.209	173.305	1.00	114.51
50	597	OE2	GLU	A	75	3.435	80.426	172.593	1.00	173.92
	598	C	GLU	A	75	2.274	83.945	168.773	1.00	48.86
	599	O	GLU	A	75	3.007	83.243	168.075	1.00	57.67
	600	N	SER	A	76	2.445	85.251	168.916	1.00	46.16
	601	CA	SER	A	76	3.520	85.981	168.260	1.00	64.43
55	602	CB	SER	A	76	3.619	87.383	168.864	1.00	108.46

	603	OG	SER	A	76	3.634	87.336	170.287	1.00	78.81
	604	C	SER	A	76	4.865	85.291	168.375	1.00	57.59
	605	O	SER	A	76	5.108	84.573	169.339	1.00	53.17
	606	N	GLU	A	77	5.728	85.486	167.379	1.00	95.85
	607	CA	GLU	A	77	7.064	84.906	167.442	1.00	46.97
	608	CB	GLU	A	77	7.893	85.273	166.211	1.00	62.29
	609	CG	GLU	A	77	7.364	84.714	164.896	1.00	130.97
	610	CD	GLU	A	77	7.571	83.215	164.760	1.00	165.99
	611	OE1	GLU	A	77	8.743	82.773	164.758	1.00	180.77
	612	OE2	GLU	A	77	6.566	82.477	164.650	1.00	160.47
	613	C	GLU	A	77	7.579	85.645	168.662	1.00	80.10
	614	O	GLU	A	77	7.229	86.804	168.880	1.00	80.13
	615	N	PRO	A	78	8.410	84.999	169.476	1.00	60.47
	616	CD	PRO	A	78	9.153	83.748	169.255	1.00	68.85
	617	CA	PRO	A	78	8.902	85.692	170.661	1.00	58.42
	618	CB	PRO	A	78	9.606	84.583	171.413	1.00	55.27
	619	CG	PRO	A	78	10.270	83.853	170.283	1.00	88.80
	620	C	PRO	A	78	9.836	86.843	170.322	1.00	68.90
	621	O	PRO	A	78	10.461	86.855	169.263	1.00	56.81
	622	N	VAL	A	79	9.914	87.809	171.231	1.00	55.88
	623	CA	VAL	A	79	10.785	88.963	171.075	1.00	53.98
	624	CB	VAL	A	79	9.980	90.251	170.992	1.00	34.06
	625	CG1	VAL	A	79	10.910	91.426	170.825	1.00	85.73
	626	CG2	VAL	A	79	9.028	90.171	169.833	1.00	97.73
	627	C	VAL	A	79	11.649	89.009	172.321	1.00	87.70
	628	O	VAL	A	79	11.119	89.113	173.433	1.00	48.94
	629	N	TYR	A	80	12.968	88.928	172.142	1.00	53.61
	630	CA	TYR	A	80	13.878	88.944	173.278	1.00	34.81
	631	CB	TYR	A	80	15.023	87.972	173.020	1.00	65.29
	632	CG	TYR	A	80	14.516	86.557	172.856	1.00	94.10
	633	CD1	TYR	A	80	14.499	85.938	171.605	1.00	67.48
	634	CE1	TYR	A	80	13.965	84.657	171.442	1.00	77.57
	635	CD2	TYR	A	80	13.989	85.856	173.947	1.00	68.38
	636	CE2	TYR	A	80	13.451	84.578	173.797	1.00	65.53
	637	CZ	TYR	A	80	13.440	83.985	172.542	1.00	93.69
	638	OH	TYR	A	80	12.885	82.733	172.385	1.00	86.31
	639	C	TYR	A	80	14.390	90.337	173.627	1.00	56.78
	640	O	TYR	A	80	14.892	91.069	172.777	1.00	63.63
	641	N	LEU	A	81	14.244	90.689	174.899	1.00	10.90
	642	CA	LEU	A	81	14.628	91.993	175.411	1.00	19.84
	643	CB	LEU	A	81	13.412	92.635	176.068	1.00	16.84
	644	CG	LEU	A	81	13.534	94.104	176.437	1.00	35.65
	645	CD1	LEU	A	81	13.214	94.911	175.209	1.00	77.33
	646	CD2	LEU	A	81	12.585	94.468	177.544	1.00	33.43
	647	C	LEU	A	81	15.748	91.903	176.441	1.00	46.78
	648	O	LEU	A	81	15.522	91.419	177.549	1.00	42.71
	649	N	GLU	A	82	16.939	92.393	176.098	1.00	20.80
	650	CA	GLU	A	82	18.070	92.348	177.024	1.00	45.93
	651	CB	GLU	A	82	19.318	91.828	176.307	1.00	24.73
	652	CG	GLU	A	82	19.115	90.473	175.638	1.00	154.76
	653	CD	GLU	A	82	20.294	90.041	174.785	1.00	173.29
	654	OE1	GLU	A	82	21.395	89.842	175.353	1.00	124.38
	655	OE2	GLU	A	82	20.112	89.903	173.550	1.00	145.47
	656	C	GLU	A	82	18.361	93.713	177.634	1.00	51.76
	657	O	GLU	A	82	18.443	94.705	176.919	1.00	33.44

	658	N	VAL	A	83	18.514	93.756	178.957	1.00	5.42
	659	CA	VAL	A	83	18.800	95.000	179.663	1.00	45.28
	660	CB	VAL	A	83	17.904	95.144	180.900	1.00	55.93
	661	CG1	VAL	A	83	18.181	96.457	181.587	1.00	84.34
5	662	CG2	VAL	A	83	16.457	95.065	180.499	1.00	47.82
	663	C	VAL	A	83	20.263	95.031	180.108	1.00	52.84
	664	O	VAL	A	83	20.694	94.195	180.901	1.00	69.13
	665	N	PHE	A	84	21.018	96.007	179.610	1.00	62.21
	666	CA	PHE	A	84	22.439	96.126	179.926	1.00	41.74
10	667	CB	PHE	A	84	23.249	96.308	178.653	1.00	33.99
	668	CG	PHE	A	84	23.117	95.196	177.675	1.00	27.72
	669	CD1	PHE	A	84	21.904	94.910	177.096	1.00	35.75
	670	CD2	PHE	A	84	24.230	94.459	177.298	1.00	63.18
	671	CE1	PHE	A	84	21.797	93.908	176.149	1.00	106.48
15	672	CE2	PHE	A	84	24.135	93.457	176.353	1.00	72.91
	673	CZ	PHE	A	84	22.917	93.179	175.776	1.00	70.31
	674	C	PHE	A	84	22.807	97.288	180.825	1.00	50.31
	675	O	PHE	A	84	21.989	98.152	181.116	1.00	51.85
	676	N	SER	A	85	24.075	97.293	181.228	1.00	58.67
20	677	CA	SER	A	85	24.676	98.342	182.054	1.00	62.35
	678	CB	SER	A	85	24.515	98.072	183.537	1.00	63.27
	679	OG	SER	A	85	25.416	98.903	184.249	1.00	42.99
	680	C	SER	A	85	26.162	98.412	181.760	1.00	20.41
	681	O	SER	A	85	26.969	97.836	182.480	1.00	71.62
25	682	N	ASP	A	86	26.503	99.124	180.694	1.00	57.01
	683	CA	ASP	A	86	27.873	99.290	180.252	1.00	18.49
	684	CB	ASP	A	86	28.179	98.274	179.158	1.00	54.07
	685	CG	ASP	A	86	29.651	98.139	178.883	1.00	94.47
	686	OD1	ASP	A	86	30.251	99.061	178.284	1.00	107.01
30	687	OD2	ASP	A	86	30.210	97.095	179.277	1.00	121.47
	688	C	ASP	A	86	28.036	100.719	179.739	1.00	38.14
	689	O	ASP	A	86	27.162	101.559	179.934	1.00	28.17
	690	N	TRP	A	87	29.143	101.007	179.080	1.00	27.21
	691	CA	TRP	A	87	29.360	102.359	178.621	1.00	5.42
35	692	CB	TRP	A	87	30.850	102.677	178.615	1.00	66.21
	693	CG	TRP	A	87	31.410	102.892	179.971	1.00	5.42
	694	CD2	TRP	A	87	31.589	104.143	180.619	1.00	22.62
	695	CE2	TRP	A	87	32.119	103.885	181.897	1.00	32.39
	696	CE3	TRP	A	87	31.356	105.467	180.243	1.00	27.34
40	697	CD1	TRP	A	87	31.831	101.934	180.863	1.00	80.10
	698	NE1	TRP	A	87	32.259	102.528	182.026	1.00	27.00
	699	CZ2	TRP	A	87	32.415	104.901	182.795	1.00	66.07
	700	CZ3	TRP	A	87	31.650	106.465	181.127	1.00	5.42
	701	CH2	TRP	A	87	32.174	106.185	182.389	1.00	51.52
45	702	C	TRP	A	87	28.756	102.597	177.260	1.00	55.21
	703	O	TRP	A	87	28.120	103.633	177.043	1.00	35.93
	704	N	LEU	A	88	28.962	101.657	176.340	1.00	11.34
	705	CA	LEU	A	88	28.380	101.771	175.005	1.00	32.20
	706	CB	LEU	A	88	29.448	101.985	173.934	1.00	5.42
50	707	CG	LEU	A	88	30.149	103.334	174.042	1.00	25.97
	708	CD1	LEU	A	88	30.908	103.647	172.772	1.00	8.11
	709	CD2	LEU	A	88	29.107	104.407	174.305	1.00	18.42
	710	C	LEU	A	88	27.579	100.530	174.686	1.00	40.80
	711	O	LEU	A	88	27.996	99.411	174.969	1.00	71.11
55	712	N	LEU	A	89	26.413	100.743	174.097	1.00	29.92

	713	CA	LEU	A	89	25.514	99.660	173.727	1.00	40.51
	714	CB	LEU	A	89	24.232	99.746	174.553	1.00	29.28
	715	CG	LEU	A	89	23.183	98.661	174.363	1.00	41.41
	716	CD1	LEU	A	89	23.364	97.607	175.406	1.00	8.36
5	717	CD2	LEU	A	89	21.807	99.251	174.519	1.00	110.85
	718	C	LEU	A	89	25.186	99.855	172.258	1.00	55.63
	719	O	LEU	A	89	24.869	100.964	171.825	1.00	37.39
	720	N	LEU	A	90	25.293	98.792	171.477	1.00	38.50
	721	CA	LEU	A	90	24.983	98.911	170.063	1.00	17.59
10	722	CB	LEU	A	90	25.917	98.066	169.229	1.00	8.86
	723	CG	LEU	A	90	25.566	98.059	167.755	1.00	23.44
	724	CD1	LEU	A	90	26.146	99.279	167.081	1.00	27.66
	725	CD2	LEU	A	90	26.117	96.794	167.137	1.00	25.45
	726	C	LEU	A	90	23.587	98.383	169.924	1.00	38.66
15	727	O	LEU	A	90	23.330	97.213	170.195	1.00	48.96
	728	N	GLN	A	91	22.681	99.251	169.505	1.00	36.75
	729	CA	GLN	A	91	21.295	98.871	169.354	1.00	8.29
	730	CB	GLN	A	91	20.401	99.929	169.966	1.00	39.59
	731	CG	GLN	A	91	20.488	100.046	171.453	1.00	5.42
20	732	CD	GLN	A	91	19.685	101.217	171.942	1.00	54.77
	733	OE1	GLN	A	91	19.702	102.288	171.325	1.00	27.61
	734	NE2	GLN	A	91	18.983	101.036	173.053	1.00	32.79
	735	C	GLN	A	91	20.927	98.713	167.903	1.00	57.80
	736	O	GLN	A	91	21.387	99.472	167.049	1.00	61.80
25	737	N	ALA	A	92	20.083	97.727	167.624	1.00	41.69
	738	CA	ALA	A	92	19.652	97.509	166.262	1.00	33.39
	739	CB	ALA	A	92	20.287	96.263	165.698	1.00	53.81
	740	C	ALA	A	92	18.147	97.400	166.213	1.00	66.17
	741	O	ALA	A	92	17.518	96.880	167.141	1.00	43.51
30	742	N	SER	A	93	17.592	97.919	165.121	1.00	31.27
	743	CA	SER	A	93	16.163	97.913	164.863	1.00	58.56
	744	CB	SER	A	93	15.890	98.616	163.541	1.00	37.57
	745	OG	SER	A	93	16.522	97.916	162.484	1.00	75.71
	746	C	SER	A	93	15.629	96.478	164.810	1.00	81.43
35	747	O	SER	A	93	14.493	96.216	165.208	1.00	48.00
	748	N	ALA	A	94	16.454	95.560	164.317	1.00	14.94
	749	CA	ALA	A	94	16.084	94.157	164.218	1.00	54.65
	750	CB	ALA	A	94	15.137	93.958	163.058	1.00	117.54
	751	C	ALA	A	94	17.323	93.302	164.028	1.00	55.96
40	752	O	ALA	A	94	18.162	93.613	163.198	1.00	62.00
	753	N	GLU	A	95	17.433	92.214	164.780	1.00	54.57
	754	CA	GLU	A	95	18.605	91.356	164.667	1.00	61.37
	755	CB	GLU	A	95	18.722	90.493	165.917	1.00	82.00
	756	CG	GLU	A	95	18.730	91.321	167.184	1.00	46.60
45	757	CD	GLU	A	95	18.734	90.472	168.427	1.00	114.77
	758	OE1	GLU	A	95	17.813	89.639	168.582	1.00	140.88
	759	OE2	GLU	A	95	19.659	90.640	169.247	1.00	105.98
	760	C	GLU	A	95	18.598	90.494	163.408	1.00	47.61
	761	O	GLU	A	95	19.650	90.135	162.888	1.00	68.07
50	762	N	VAL	A	96	17.407	90.163	162.926	1.00	79.01
	763	CA	VAL	A	96	17.246	89.377	161.703	1.00	53.09
	764	CB	VAL	A	96	16.572	88.026	161.974	1.00	60.34
	765	CG1	VAL	A	96	16.439	87.269	160.687	1.00	66.62
	766	CG2	VAL	A	96	17.384	87.219	162.972	1.00	75.27
55	767	C	VAL	A	96	16.348	90.214	160.801	1.00	37.17

	768	O	VAL	A	96	15.182	90.453	161.107	1.00	67.51
	769	N	VAL	A	97	16.900	90.673	159.692	1.00	31.53
	770	CA	VAL	A	97	16.164	91.532	158.786	1.00	61.27
	771	CB	VAL	A	97	16.945	92.851	158.561	1.00	37.63
5	772	CG1	VAL	A	97	16.712	93.382	157.165	1.00	101.90
	773	CG2	VAL	A	97	16.501	93.882	159.579	1.00	109.18
	774	C	VAL	A	97	15.894	90.875	157.450	1.00	74.73
	775	O	VAL	A	97	16.828	90.509	156.745	1.00	91.83
	776	N	MET	A	98	14.615	90.734	157.103	1.00	107.16
10	777	CA	MET	A	98	14.229	90.126	155.835	1.00	85.06
	778	CB	MET	A	98	12.701	90.028	155.717	1.00	152.68
	779	CG	MET	A	98	12.042	89.134	156.758	1.00	194.20
	780	SD	MET	A	98	10.239	89.149	156.658	1.00	216.44
	781	CE	MET	A	98	9.857	90.576	157.704	1.00	214.75
15	782	C	MET	A	98	14.778	90.978	154.699	1.00	101.32
	783	O	MET	A	98	14.724	92.203	154.747	1.00	54.34
	784	N	GLU	A	99	15.315	90.312	153.684	1.00	129.05
	785	CA	GLU	A	99	15.895	90.956	152.506	1.00	108.86
	786	CB	GLU	A	99	15.975	89.918	151.373	1.00	189.93
20	787	CG	GLU	A	99	16.759	90.309	150.123	1.00	203.35
	788	CD	GLU	A	99	16.928	89.132	149.164	1.00	206.77
	789	OE1	GLU	A	99	15.908	88.496	148.810	1.00	194.67
	790	OE2	GLU	A	99	18.079	88.844	148.765	1.00	186.48
	791	C	GLU	A	99	15.083	92.177	152.061	1.00	72.06
25	792	O	GLU	A	99	13.856	92.132	152.005	1.00	110.93
	793	N	GLY	A	100	15.770	93.271	151.758	1.00	62.36
	794	CA	GLY	A	100	15.080	94.470	151.312	1.00	77.49
	795	C	GLY	A	100	14.648	95.464	152.380	1.00	106.99
	796	O	GLY	A	100	14.773	96.675	152.180	1.00	142.90
30	797	N	GLN	A	101	14.134	94.967	153.505	1.00	76.10
	798	CA	GLN	A	101	13.691	95.830	154.606	1.00	99.54
	799	CB	GLN	A	101	13.125	94.970	155.749	1.00	118.17
	800	CG	GLN	A	101	11.942	94.075	155.371	1.00	127.37
	801	CD	GLN	A	101	10.670	94.847	155.045	1.00	143.15
35	802	OE1	GLN	A	101	10.628	96.072	155.148	1.00	128.68
	803	NE2	GLN	A	101	9.622	94.125	154.657	1.00	171.66
	804	C	GLN	A	101	14.821	96.737	155.149	1.00	80.68
	805	O	GLN	A	101	16.007	96.446	154.978	1.00	81.82
	806	N	PRO	A	102	14.461	97.854	155.803	1.00	39.03
40	807	CD	PRO	A	102	13.105	98.404	155.959	1.00	80.04
	808	CA	PRO	A	102	15.446	98.779	156.359	1.00	46.08
	809	CB	PRO	A	102	14.633	100.039	156.586	1.00	68.48
	810	CG	PRO	A	102	13.316	99.493	156.982	1.00	39.46
	811	C	PRO	A	102	16.106	98.283	157.645	1.00	68.21
45	812	O	PRO	A	102	15.560	97.432	158.365	1.00	33.76
	813	N	LEU	A	103	17.280	98.847	157.924	1.00	47.86
	814	CA	LEU	A	103	18.070	98.496	159.093	1.00	42.26
	815	CB	LEU	A	103	19.201	97.587	158.673	1.00	5.42
	816	CG	LEU	A	103	20.077	97.146	159.825	1.00	53.71
50	817	CD1	LEU	A	103	19.245	96.340	160.809	1.00	30.09
	818	CD2	LEU	A	103	21.239	96.342	159.271	1.00	40.52
	819	C	LEU	A	103	18.656	99.713	159.791	1.00	39.88
	820	O	LEU	A	103	19.091	100.667	159.149	1.00	48.87
	821	N	PHE	A	104	18.690	99.675	161.113	1.00	16.90
55	822	CA	PHE	A	104	19.229	100.796	161.853	1.00	47.53

	823	CB	PHE	A	104	18.107	101.655	162.406	1.00	17.73
	824	CG	PHE	A	104	17.195	102.171	161.361	1.00	55.90
	825	CD1	PHE	A	104	15.965	101.566	161.139	1.00	15.89
	826	CD2	PHE	A	104	17.569	103.257	160.577	1.00	76.37
5	827	CE1	PHE	A	104	15.105	102.040	160.146	1.00	68.24
	828	CE2	PHE	A	104	16.719	103.743	159.579	1.00	94.38
	829	CZ	PHE	A	104	15.481	103.133	159.363	1.00	50.60
	830	C	PHE	A	104	20.150	100.419	162.978	1.00	42.37
	831	O	PHE	A	104	19.834	99.593	163.832	1.00	47.93
10	832	N	LEU	A	105	21.306	101.049	162.970	1.00	26.80
	833	CA	LEU	A	105	22.277	100.811	163.995	1.00	33.05
	834	CB	LEU	A	105	23.609	100.437	163.362	1.00	47.90
	835	CG	LEU	A	105	23.596	99.200	162.464	1.00	47.60
	836	CD1	LEU	A	105	24.941	99.044	161.777	1.00	83.01
15	837	CD2	LEU	A	105	23.285	97.976	163.291	1.00	13.75
	838	C	LEU	A	105	22.391	102.129	164.720	1.00	52.31
	839	O	LEU	A	105	22.230	103.192	164.123	1.00	53.94
	840	N	ARG	A	106	22.676	102.055	166.010	1.00	21.83
	841	CA	ARG	A	106	22.819	103.239	166.837	1.00	41.63
20	842	CB	ARG	A	106	21.456	103.568	167.438	1.00	23.32
	843	CG	ARG	A	106	21.448	104.739	168.369	1.00	51.86
	844	CD	ARG	A	106	20.098	104.857	169.030	1.00	30.81
	845	NE	ARG	A	106	20.162	105.533	170.318	1.00	31.36
	846	CZ	ARG	A	106	19.100	105.803	171.065	1.00	52.13
25	847	NH1	ARG	A	106	17.892	105.459	170.642	1.00	93.33
	848	NH2	ARG	A	106	19.240	106.401	172.241	1.00	34.31
	849	C	ARG	A	106	23.838	102.977	167.956	1.00	57.42
	850	O	ARG	A	106	23.716	101.991	168.685	1.00	30.30
	851	N	CYS	A	107	24.866	103.815	168.077	1.00	24.37
30	852	CA	CYS	A	107	25.807	103.616	169.176	1.00	42.73
	853	C	CYS	A	107	25.176	104.464	170.251	1.00	44.66
	854	O	CYS	A	107	25.065	105.682	170.102	1.00	52.70
	855	CB	CYS	A	107	27.216	104.119	168.858	1.00	5.42
	856	SG	CYS	A	107	28.525	103.331	169.872	1.00	82.53
35	857	N	HIS	A	108	24.717	103.804	171.311	1.00	11.14
	858	CA	HIS	A	108	24.045	104.487	172.398	1.00	21.95
	859	CB	HIS	A	108	22.770	103.755	172.765	1.00	13.74
	860	CG	HIS	A	108	21.954	104.478	173.783	1.00	50.61
	861	CD2	HIS	A	108	21.270	104.037	174.864	1.00	13.51
40	862	ND1	HIS	A	108	21.783	105.845	173.750	1.00	39.22
	863	CE1	HIS	A	108	21.030	106.213	174.769	1.00	67.80
	864	NE2	HIS	A	108	20.706	105.135	175.460	1.00	46.62
	865	C	HIS	A	108	24.898	104.633	173.634	1.00	52.09
	866	O	HIS	A	108	25.330	103.648	174.220	1.00	15.69
45	867	N	GLY	A	109	25.122	105.874	174.047	1.00	37.30
	868	CA	GLY	A	109	25.950	106.085	175.212	1.00	36.86
	869	C	GLY	A	109	25.165	106.142	176.498	1.00	46.50
	870	O	GLY	A	109	24.159	106.838	176.579	1.00	42.12
	871	N	TRP	A	110	25.641	105.412	177.501	1.00	7.94
50	872	CA	TRP	A	110	25.033	105.365	178.824	1.00	30.83
	873	CB	TRP	A	110	26.075	104.901	179.816	1.00	5.42
	874	CG	TRP	A	110	25.536	104.902	181.182	1.00	67.67
	875	CD2	TRP	A	110	24.735	103.879	181.772	1.00	56.37
	876	CE2	TRP	A	110	24.444	104.283	183.085	1.00	18.12
55	877	CE3	TRP	A	110	24.239	102.654	181.316	1.00	81.28

	878	CD1	TRP	A	110	25.692	105.866	182.129	1.00	37.15
	879	NE1	TRP	A	110	25.039	105.500	183.283	1.00	90.09
	880	CZ2	TRP	A	110	23.685	103.510	183.944	1.00	53.89
	881	CZ3	TRP	A	110	23.484	101.886	182.176	1.00	86.79
5	882	CH2	TRP	A	110	23.216	102.317	183.476	1.00	35.12
	883	C	TRP	A	110	24.430	106.697	179.304	1.00	25.46
	884	O	TRP	A	110	24.984	107.758	179.042	1.00	34.32
	885	N	ARG	A	111	23.324	106.639	180.045	1.00	9.65
	886	CA	ARG	A	111	22.640	107.855	180.509	1.00	64.56
10	887	CB	ARG	A	111	23.299	108.434	181.778	1.00	5.57
	888	CG	ARG	A	111	23.045	107.558	183.026	1.00	122.90
	889	CD	ARG	A	111	23.274	108.250	184.384	1.00	92.09
	890	NE	ARG	A	111	22.026	108.704	185.001	1.00	66.00
	891	CZ	ARG	A	111	21.283	109.706	184.540	1.00	111.74
15	892	NH1	ARG	A	111	21.659	110.370	183.454	1.00	85.41
	893	NH2	ARG	A	111	20.159	110.045	185.159	1.00	106.66
	894	C	ARG	A	111	22.590	108.889	179.383	1.00	25.39
	895	O	ARG	A	111	22.455	110.096	179.584	1.00	35.74
	896	N	ASN	A	112	22.668	108.367	178.176	1.00	22.55
20	897	CA	ASN	A	112	22.638	109.160	176.979	1.00	55.36
	898	CB	ASN	A	112	21.259	109.811	176.809	1.00	23.18
	899	CG	ASN	A	112	20.903	110.048	175.338	1.00	99.46
	900	OD1	ASN	A	112	21.105	109.180	174.484	1.00	76.98
	901	ND2	ASN	A	112	20.363	111.225	175.042	1.00	120.92
25	902	C	ASN	A	112	23.759	110.186	177.006	1.00	30.60
	903	O	ASN	A	112	23.623	111.301	176.503	1.00	78.43
	904	N	TRP	A	113	24.884	109.793	177.590	1.00	28.24
	905	CA	TRP	A	113	26.034	110.674	177.632	1.00	46.75
	906	CB	TRP	A	113	27.127	110.128	178.532	1.00	19.32
30	907	CG	TRP	A	113	26.882	110.334	179.969	1.00	11.92
	908	CD2	TRP	A	113	27.516	109.646	181.050	1.00	26.29
	909	CE2	TRP	A	113	27.000	110.174	182.242	1.00	5.42
	910	CE3	TRP	A	113	28.477	108.636	181.124	1.00	22.82
	911	CD1	TRP	A	113	26.037	111.226	180.528	1.00	35.81
35	912	NE1	TRP	A	113	26.095	111.138	181.899	1.00	39.35
	913	CZ2	TRP	A	113	27.411	109.724	183.501	1.00	42.09
	914	CZ3	TRP	A	113	28.886	108.191	182.375	1.00	13.91
	915	CH2	TRP	A	113	28.355	108.733	183.542	1.00	5.42
	916	C	TRP	A	113	26.585	110.818	176.232	1.00	39.58
40	917	O	TRP	A	113	26.479	109.921	175.397	1.00	56.66
	918	N	ASP	A	114	27.174	111.970	175.983	1.00	40.70
	919	CA	ASP	A	114	27.749	112.254	174.696	1.00	44.29
	920	CB	ASP	A	114	28.223	113.698	174.678	1.00	49.96
	921	CG	ASP	A	114	27.094	114.663	174.860	1.00	31.77
45	922	OD1	ASP	A	114	26.224	114.722	173.964	1.00	75.41
	923	OD2	ASP	A	114	27.072	115.349	175.897	1.00	54.49
	924	C	ASP	A	114	28.910	111.324	174.393	1.00	58.03
	925	O	ASP	A	114	29.718	111.023	175.268	1.00	34.68
	926	N	VAL	A	115	28.967	110.858	173.148	1.00	30.06
50	927	CA	VAL	A	115	30.048	109.990	172.687	1.00	31.75
	928	CB	VAL	A	115	29.579	108.551	172.316	1.00	9.73
	929	CG1	VAL	A	115	30.611	107.900	171.442	1.00	60.47
	930	CG2	VAL	A	115	29.447	107.693	173.535	1.00	5.42
	931	C	VAL	A	115	30.623	110.612	171.426	1.00	24.47
55	932	O	VAL	A	115	29.931	110.735	170.423	1.00	47.65

	933	N	TYR	A	116	31.886	111.012	171.465	1.00	30.10
	934	CA	TYR	A	116	32.479	111.602	170.279	1.00	17.95
	935	CB	TYR	A	116	33.256	112.865	170.637	1.00	61.65
	936	CG	TYR	A	116	32.427	113.950	171.286	1.00	16.29
5	937	CD1	TYR	A	116	32.051	113.862	172.611	1.00	20.60
	938	CE1	TYR	A	116	31.273	114.839	173.205	1.00	49.07
	939	CD2	TYR	A	116	32.004	115.049	170.560	1.00	22.42
	940	CE2	TYR	A	116	31.227	116.031	171.138	1.00	73.73
	941	CZ	TYR	A	116	30.864	115.920	172.460	1.00	14.21
10	942	OH	TYR	A	116	30.091	116.898	173.033	1.00	94.60
	943	C	TYR	A	116	33.391	110.599	169.588	1.00	45.63
	944	O	TYR	A	116	33.850	109.628	170.205	1.00	28.02
	945	N	LYS	A	117	33.636	110.842	168.302	1.00	6.49
	946	CA	LYS	A	117	34.479	109.975	167.479	1.00	35.81
15	947	CB	LYS	A	117	35.937	110.034	167.974	1.00	21.69
	948	CG	LYS	A	117	36.715	111.214	167.404	1.00	9.02
	949	CD	LYS	A	117	37.800	111.699	168.323	1.00	36.98
	950	CE	LYS	A	117	38.449	112.977	167.779	1.00	25.36
	951	NZ	LYS	A	117	39.653	113.406	168.569	1.00	25.77
20	952	C	LYS	A	117	33.962	108.543	167.472	1.00	7.50
	953	O	LYS	A	117	34.687	107.595	167.749	1.00	52.96
	954	N	VAL	A	118	32.693	108.398	167.136	1.00	46.87
	955	CA	VAL	A	118	32.045	107.102	167.109	1.00	14.75
	956	CB	VAL	A	118	30.540	107.259	167.103	1.00	8.67
25	957	CG1	VAL	A	118	29.897	105.947	167.298	1.00	27.58
	958	CG2	VAL	A	118	30.122	108.227	168.165	1.00	69.02
	959	C	VAL	A	118	32.404	106.398	165.829	1.00	30.61
	960	O	VAL	A	118	32.314	106.981	164.755	1.00	19.62
	961	N	ILE	A	119	32.821	105.148	165.939	1.00	26.47
30	962	CA	ILE	A	119	33.130	104.369	164.753	1.00	43.90
	963	CB	ILE	A	119	34.604	104.042	164.634	1.00	35.19
	964	CG2	ILE	A	119	34.809	103.093	163.482	1.00	23.28
	965	CG1	ILE	A	119	35.406	105.305	164.379	1.00	48.21
	966	CD1	ILE	A	119	36.855	105.042	164.194	1.00	13.69
35	967	C	ILE	A	119	32.391	103.054	164.815	1.00	59.19
	968	O	ILE	A	119	32.403	102.371	165.840	1.00	67.21
	969	N	TYR	A	120	31.743	102.698	163.720	1.00	17.08
	970	CA	TYR	A	120	31.023	101.445	163.679	1.00	30.07
	971	CB	TYR	A	120	29.692	101.622	162.976	1.00	13.53
40	972	CG	TYR	A	120	28.673	102.393	163.755	1.00	11.12
	973	CD1	TYR	A	120	28.517	103.760	163.585	1.00	17.26
	974	CE1	TYR	A	120	27.509	104.438	164.227	1.00	5.42
	975	CD2	TYR	A	120	27.806	101.737	164.599	1.00	25.25
	976	CE2	TYR	A	120	26.803	102.398	165.243	1.00	15.18
45	977	CZ	TYR	A	120	26.647	103.740	165.056	1.00	46.64
	978	OH	TYR	A	120	25.595	104.357	165.687	1.00	52.40
	979	C	TYR	A	120	31.864	100.435	162.917	1.00	68.41
	980	O	TYR	A	120	32.395	100.743	161.850	1.00	28.49
	981	N	TYR	A	121	31.991	99.229	163.466	1.00	51.87
50	982	CA	TYR	A	121	32.769	98.187	162.811	1.00	25.77
	983	CB	TYR	A	121	33.826	97.598	163.747	1.00	54.55
	984	CG	TYR	A	121	34.978	98.529	164.015	1.00	8.44
	985	CD1	TYR	A	121	34.991	99.343	165.133	1.00	59.81
	986	CE1	TYR	A	121	36.010	100.254	165.343	1.00	105.65
55	987	CD2	TYR	A	121	36.022	98.645	163.112	1.00	79.41

	988	CE2	TYR	A	121	37.047	99.558	163.313	1.00	65.81
	989	CZ	TYR	A	121	37.031	100.355	164.426	1.00	13.26
	990	OH	TYR	A	121	38.023	101.270	164.627	1.00	74.37
	991	C	TYR	A	121	31.882	97.078	162.315	1.00	71.36
	992	O	TYR	A	121	30.877	96.730	162.942	1.00	47.92
	993	N	LYS	A	122	32.271	96.533	161.171	1.00	48.07
	994	CA	LYS	A	122	31.550	95.452	160.537	1.00	62.27
	995	CB	LYS	A	122	30.826	95.951	159.290	1.00	82.65
	996	CG	LYS	A	122	30.100	94.878	158.498	1.00	56.59
	997	CD	LYS	A	122	29.471	95.512	157.272	1.00	114.33
	998	CE	LYS	A	122	28.714	94.519	156.423	1.00	90.73
	999	NZ	LYS	A	122	28.074	95.227	155.275	1.00	102.70
	1000	C	LYS	A	122	32.575	94.415	160.149	1.00	51.78
	1001	O	LYS	A	122	33.377	94.622	159.236	1.00	58.80
	1002	N	ASP	A	123	32.544	93.296	160.855	1.00	69.12
	1003	CA	ASP	A	123	33.464	92.205	160.595	1.00	94.48
	1004	CB	ASP	A	123	33.175	91.559	159.230	1.00	102.02
	1005	CG	ASP	A	123	31.808	90.890	159.170	1.00	106.91
	1006	OD1	ASP	A	123	31.492	90.097	160.087	1.00	80.34
	1007	OD2	ASP	A	123	31.056	91.152	158.201	1.00	91.23
	1008	C	ASP	A	123	34.887	92.725	160.633	1.00	42.69
	1009	O	ASP	A	123	35.642	92.572	159.682	1.00	80.39
	1010	N	GLY	A	124	35.240	93.353	161.741	1.00	42.82
	1011	CA	GLY	A	124	36.585	93.862	161.892	1.00	58.87
	1012	C	GLY	A	124	36.987	94.991	160.970	1.00	46.57
	1013	O	GLY	A	124	38.117	95.452	161.037	1.00	81.66
	1014	N	GLU	A	125	36.092	95.440	160.102	1.00	57.50
	1015	CA	GLU	A	125	36.434	96.544	159.211	1.00	57.91
	1016	CB	GLU	A	125	35.933	96.298	157.791	1.00	140.86
	1017	CG	GLU	A	125	36.385	95.024	157.122	1.00	176.84
	1018	CD	GLU	A	125	35.928	94.972	155.677	1.00	189.28
	1019	OE1	GLU	A	125	34.704	95.097	155.438	1.00	165.09
	1020	OE2	GLU	A	125	36.794	94.814	154.785	1.00	176.42
	1021	C	GLU	A	125	35.779	97.823	159.701	1.00	49.34
	1022	O	GLU	A	125	34.723	97.791	160.328	1.00	70.32
	1023	N	ALA	A	126	36.400	98.953	159.400	1.00	54.71
	1024	CA	ALA	A	126	35.850	100.237	159.793	1.00	36.67
	1025	CB	ALA	A	126	36.928	101.281	159.793	1.00	40.73
	1026	C	ALA	A	126	34.775	100.614	158.799	1.00	28.44
	1027	O	ALA	A	126	35.074	100.962	157.660	1.00	49.69
	1028	N	LEU	A	127	33.523	100.557	159.235	1.00	38.11
	1029	CA	LEU	A	127	32.412	100.888	158.365	1.00	35.41
	1030	CB	LEU	A	127	31.141	100.219	158.880	1.00	24.22
	1031	CG	LEU	A	127	29.869	100.320	158.045	1.00	33.49
	1032	CD1	LEU	A	127	30.194	100.562	156.587	1.00	56.43
	1033	CD2	LEU	A	127	29.077	99.041	158.237	1.00	47.01
	1034	C	LEU	A	127	32.226	102.393	158.225	1.00	30.36
	1035	O	LEU	A	127	32.289	102.902	157.118	1.00	60.67
	1036	N	LYS	A	128	32.014	103.108	159.331	1.00	28.99
	1037	CA	LYS	A	128	31.836	104.566	159.273	1.00	33.91
	1038	CB	LYS	A	128	30.366	104.916	159.041	1.00	38.64
	1039	CG	LYS	A	128	30.131	106.337	158.560	1.00	15.25
	1040	CD	LYS	A	128	28.691	106.479	158.073	1.00	113.62
	1041	CE	LYS	A	128	28.493	107.706	157.188	1.00	123.73
	1042	NZ	LYS	A	128	27.202	107.663	156.419	1.00	121.55

	1043	C	LYS	A	128	32.317	105.281	160.530	1.00	52.08
	1044	O	LYS	A	128	32.077	104.819	161.647	1.00	65.58
	1045	N	TYR	A	129	33.011	106.401	160.343	1.00	31.59
	1046	CA	TYR	A	129	33.509	107.213	161.459	1.00	36.12
5	1047	CB	TYR	A	129	35.037	107.317	161.450	1.00	18.41
	1048	CG	TYR	A	129	35.608	108.593	162.076	1.00	5.42
	1049	CD1	TYR	A	129	36.136	108.584	163.348	1.00	44.66
	1050	CE1	TYR	A	129	36.655	109.734	163.923	1.00	33.53
	1051	CD2	TYR	A	129	35.619	109.804	161.386	1.00	23.01
10	1052	CE2	TYR	A	129	36.141	110.962	161.959	1.00	5.42
	1053	CZ	TYR	A	129	36.653	110.910	163.229	1.00	39.44
	1054	OH	TYR	A	129	37.173	112.024	163.828	1.00	26.10
	1055	C	TYR	A	129	32.942	108.600	161.285	1.00	49.76
	1056	O	TYR	A	129	32.749	109.063	160.160	1.00	59.27
15	1057	N	TRP	A	130	32.696	109.263	162.401	1.00	24.05
	1058	CA	TRP	A	130	32.177	110.612	162.378	1.00	29.33
	1059	CB	TRP	A	130	30.653	110.586	162.363	1.00	41.56
	1060	CG	TRP	A	130	30.067	111.918	162.139	1.00	34.89
	1061	CD2	TRP	A	130	30.311	112.772	161.028	1.00	20.74
20	1062	CE2	TRP	A	130	29.535	113.931	161.210	1.00	30.33
	1063	CE3	TRP	A	130	31.109	112.673	159.893	1.00	40.31
	1064	CD1	TRP	A	130	29.177	112.571	162.937	1.00	110.45
	1065	NE1	TRP	A	130	28.849	113.786	162.385	1.00	102.78
	1066	CZ2	TRP	A	130	29.540	114.979	160.298	1.00	108.00
25	1067	CZ3	TRP	A	130	31.112	113.715	158.989	1.00	14.76
	1068	CH2	TRP	A	130	30.337	114.847	159.193	1.00	47.04
	1069	C	TRP	A	130	32.700	111.316	163.628	1.00	59.29
	1070	O	TRP	A	130	32.949	110.683	164.672	1.00	22.78
	1071	N	TYR	A	131	32.875	112.625	163.529	1.00	5.42
30	1072	CA	TYR	A	131	33.406	113.361	164.664	1.00	43.44
	1073	CB	TYR	A	131	33.533	114.856	164.336	1.00	20.56
	1074	CG	TYR	A	131	34.068	115.149	162.945	1.00	6.92
	1075	CD1	TYR	A	131	33.219	115.167	161.850	1.00	40.67
	1076	CE1	TYR	A	131	33.693	115.445	160.573	1.00	38.77
35	1077	CD2	TYR	A	131	35.422	115.414	162.728	1.00	31.32
	1078	CE2	TYR	A	131	35.908	115.689	161.455	1.00	16.93
	1079	CZ	TYR	A	131	35.034	115.708	160.384	1.00	49.10
	1080	OH	TYR	A	131	35.486	116.022	159.126	1.00	47.13
	1081	C	TYR	A	131	32.535	113.175	165.887	1.00	28.76
40	1082	O	TYR	A	131	33.030	113.124	167.015	1.00	36.69
	1083	N	GLU	A	132	31.232	113.060	165.646	1.00	21.77
	1084	CA	GLU	A	132	30.249	112.914	166.710	1.00	35.07
	1085	CB	GLU	A	132	29.315	114.113	166.691	1.00	5.42
	1086	CG	GLU	A	132	29.974	115.382	167.187	1.00	32.08
45	1087	CD	GLU	A	132	30.190	116.404	166.099	1.00	77.18
	1088	OE1	GLU	A	132	29.797	116.117	164.946	1.00	30.77
	1089	OE2	GLU	A	132	30.748	117.487	166.408	1.00	46.31
	1090	C	GLU	A	132	29.443	111.640	166.590	1.00	26.10
	1091	O	GLU	A	132	29.647	110.866	165.680	1.00	44.94
50	1092	N	ASN	A	133	28.529	111.413	167.518	1.00	42.20
	1093	CA	ASN	A	133	27.708	110.215	167.468	1.00	5.42
	1094	CB	ASN	A	133	26.848	110.093	168.700	1.00	21.79
	1095	CG	ASN	A	133	26.554	108.677	169.032	1.00	28.76
	1096	OD1	ASN	A	133	26.285	107.878	168.144	1.00	22.35
55	1097	ND2	ASN	A	133	26.603	108.344	170.318	1.00	74.20

	1098	C	ASN	A	133	26.811	110.371	166.285	1.00	11.75
	1099	O	ASN	A	133	26.539	111.500	165.877	1.00	33.27
	1100	N	HIS	A	134	26.338	109.252	165.744	1.00	5.42
	1101	CA	HIS	A	134	25.485	109.278	164.559	1.00	30.76
5	1102	CB	HIS	A	134	26.317	109.594	163.321	1.00	50.57
	1103	CG	HIS	A	134	27.435	108.627	163.085	1.00	21.60
	1104	CD2	HIS	A	134	27.659	107.753	162.077	1.00	76.57
	1105	ND1	HIS	A	134	28.481	108.468	163.965	1.00	61.39
	1106	CE1	HIS	A	134	29.300	107.539	163.512	1.00	26.75
10	1107	NE2	HIS	A	134	28.823	107.088	162.368	1.00	47.66
	1108	C	HIS	A	134	24.864	107.917	164.384	1.00	24.80
	1109	O	HIS	A	134	25.441	106.932	164.821	1.00	42.22
	1110	N	ALA	A	135	23.706	107.844	163.733	1.00	51.38
	1111	CA	ALA	A	135	23.053	106.550	163.541	1.00	50.85
15	1112	CB	ALA	A	135	21.551	106.694	163.647	1.00	25.54
	1113	C	ALA	A	135	23.428	106.009	162.188	1.00	30.29
	1114	O	ALA	A	135	23.718	106.776	161.277	1.00	75.67
	1115	N	ILE	A	136	23.448	104.687	162.064	1.00	48.62
	1116	CA	ILE	A	136	23.789	104.039	160.802	1.00	34.81
20	1117	CB	ILE	A	136	24.593	102.724	160.998	1.00	59.15
	1118	CG2	ILE	A	136	24.856	102.076	159.664	1.00	5.42
	1119	CG1	ILE	A	136	25.942	103.004	161.664	1.00	55.26
	1120	CD1	ILE	A	136	26.878	103.861	160.822	1.00	92.37
	1121	C	ILE	A	136	22.450	103.677	160.245	1.00	36.44
25	1122	O	ILE	A	136	21.735	102.876	160.844	1.00	40.66
	1123	N	SER	A	137	22.104	104.274	159.110	1.00	71.47
	1124	CA	SER	A	137	20.813	104.022	158.477	1.00	77.26
	1125	CB	SER	A	137	20.064	105.335	158.248	1.00	65.71
	1126	OG	SER	A	137	19.920	106.070	159.449	1.00	92.34
30	1127	C	SER	A	137	20.952	103.301	157.150	1.00	55.90
	1128	O	SER	A	137	21.323	103.895	156.137	1.00	68.68
	1129	N	ILE	A	138	20.650	102.012	157.164	1.00	62.52
	1130	CA	ILE	A	138	20.717	101.202	155.961	1.00	61.92
	1131	CB	ILE	A	138	21.275	99.827	156.270	1.00	45.81
35	1132	CG2	ILE	A	138	21.312	98.999	155.015	1.00	82.72
	1133	CG1	ILE	A	138	22.673	99.965	156.863	1.00	76.93
	1134	CD1	ILE	A	138	23.230	98.666	157.415	1.00	63.77
	1135	C	ILE	A	138	19.312	101.056	155.375	1.00	89.17
	1136	O	ILE	A	138	18.525	100.208	155.807	1.00	38.61
40	1137	N	THR	A	139	19.023	101.907	154.393	1.00	109.71
	1138	CA	THR	A	139	17.742	101.970	153.689	1.00	95.12
	1139	CB	THR	A	139	17.840	102.956	152.539	1.00	101.48
	1140	OG1	THR	A	139	19.147	102.850	151.946	1.00	113.46
	1141	CG2	THR	A	139	17.596	104.370	153.036	1.00	70.63
45	1142	C	THR	A	139	17.208	100.663	153.123	1.00	107.81
	1143	O	THR	A	139	16.044	100.321	153.342	1.00	75.17
	1144	N	ASN	A	140	18.048	99.955	152.370	1.00	119.96
	1145	CA	ASN	A	140	17.660	98.679	151.769	1.00	77.07
	1146	CB	ASN	A	140	17.495	98.828	150.257	1.00	128.43
50	1147	CG	ASN	A	140	16.465	99.873	149.888	1.00	149.94
	1148	OD1	ASN	A	140	15.330	99.840	150.365	1.00	158.03
	1149	ND2	ASN	A	140	16.855	100.810	149.029	1.00	147.94
	1150	C	ASN	A	140	18.691	97.603	152.065	1.00	96.65
	1151	O	ASN	A	140	19.802	97.615	151.527	1.00	86.22
55	1152	N	ALA	A	141	18.308	96.666	152.922	1.00	38.12

	1153	CA	ALA	A	141	19.196	95.588	153.316	1.00	94.25
	1154	CB	ALA	A	141	18.435	94.592	154.164	1.00	53.34
	1155	C	ALA	A	141	19.844	94.885	152.126	1.00	79.54
	1156	O	ALA	A	141	19.409	95.042	150.987	1.00	77.48
5	1157	N	ALA	A	142	20.889	94.112	152.406	1.00	90.86
	1158	CA	ALA	A	142	21.617	93.374	151.383	1.00	76.61
	1159	CB	ALA	A	142	22.683	94.261	150.761	1.00	121.64
	1160	C	ALA	A	142	22.260	92.150	152.022	1.00	74.42
	1161	O	ALA	A	142	21.987	91.843	153.176	1.00	111.57
10	1162	N	VAL	A	143	23.114	91.458	151.274	1.00	108.94
	1163	CA	VAL	A	143	23.795	90.262	151.768	1.00	116.05
	1164	CB	VAL	A	143	24.071	89.259	150.609	1.00	186.06
	1165	CG1	VAL	A	143	24.745	89.977	149.434	1.00	191.15
	1166	CG2	VAL	A	143	24.948	88.112	151.109	1.00	210.48
15	1167	C	VAL	A	143	25.115	90.625	152.440	1.00	117.36
	1168	O	VAL	A	143	25.496	90.038	153.456	1.00	94.53
	1169	N	GLU	A	144	25.813	91.588	151.853	1.00	118.63
	1170	CA	GLU	A	144	27.080	92.049	152.389	1.00	89.21
	1171	CB	GLU	A	144	27.662	93.116	151.474	1.00	107.26
20	1172	CG	GLU	A	144	26.646	94.190	151.126	1.00	114.43
	1173	CD	GLU	A	144	27.276	95.427	150.535	1.00	150.22
	1174	OE1	GLU	A	144	28.027	95.290	149.546	1.00	173.95
	1175	OE2	GLU	A	144	27.015	96.535	151.056	1.00	124.46
	1176	C	GLU	A	144	26.810	92.655	153.756	1.00	100.45
25	1177	O	GLU	A	144	27.642	92.564	154.661	1.00	113.43
	1178	N	ASP	A	145	25.635	93.269	153.891	1.00	69.60
	1179	CA	ASP	A	145	25.231	93.912	155.135	1.00	62.50
	1180	CB	ASP	A	145	23.927	94.699	154.945	1.00	35.86
	1181	CG	ASP	A	145	24.153	96.053	154.284	1.00	114.94
30	1182	OD1	ASP	A	145	25.187	96.694	154.585	1.00	110.06
	1183	OD2	ASP	A	145	23.295	96.481	153.477	1.00	95.06
	1184	C	ASP	A	145	25.102	93.000	156.350	1.00	52.48
	1185	O	ASP	A	145	24.774	93.466	157.435	1.00	45.00
	1186	N	SER	A	146	25.339	91.706	156.189	1.00	41.79
35	1187	CA	SER	A	146	25.277	90.834	157.347	1.00	56.05
	1188	CB	SER	A	146	24.848	89.426	156.965	1.00	71.16
	1189	OG	SER	A	146	23.440	89.341	156.889	1.00	94.99
	1190	C	SER	A	146	26.658	90.785	157.969	1.00	69.92
	1191	O	SER	A	146	27.594	91.438	157.498	1.00	69.56
40	1192	N	GLY	A	147	26.787	90.000	159.026	1.00	47.55
	1193	CA	GLY	A	147	28.067	89.894	159.693	1.00	98.06
	1194	C	GLY	A	147	27.921	90.473	161.076	1.00	50.55
	1195	O	GLY	A	147	26.837	90.915	161.439	1.00	81.86
	1196	N	THR	A	148	28.996	90.477	161.852	1.00	54.75
45	1197	CA	THR	A	148	28.923	91.009	163.199	1.00	47.04
	1198	CB	THR	A	148	29.784	90.196	164.160	1.00	5.42
	1199	OG1	THR	A	148	31.016	90.882	164.383	1.00	70.34
	1200	CG2	THR	A	148	30.080	88.841	163.572	1.00	60.94
	1201	C	THR	A	148	29.380	92.461	163.255	1.00	42.31
50	1202	O	THR	A	148	30.388	92.827	162.656	1.00	52.98
	1203	N	TYR	A	149	28.623	93.285	163.976	1.00	52.62
	1204	CA	TYR	A	149	28.950	94.695	164.128	1.00	25.73
	1205	CB	TYR	A	149	27.786	95.584	163.725	1.00	15.90
	1206	CG	TYR	A	149	27.380	95.588	162.288	1.00	26.25
55	1207	CD1	TYR	A	149	26.653	94.538	161.750	1.00	26.15

	1208	CE1	TYR	A	149	26.201	94.583	160.445	1.00	48.47
	1209	CD2	TYR	A	149	27.651	96.686	161.482	1.00	25.17
	1210	CE2	TYR	A	149	27.206	96.742	160.182	1.00	41.99
	1211	CZ	TYR	A	149	26.483	95.688	159.666	1.00	45.90
5	1212	OH	TYR	A	149	26.063	95.738	158.359	1.00	54.85
	1213	C	TYR	A	149	29.266	95.050	165.577	1.00	59.07
	1214	O	TYR	A	149	29.000	94.275	166.503	1.00	29.97
	1215	N	TYR	A	150	29.820	96.244	165.757	1.00	27.86
	1216	CA	TYR	A	150	30.127	96.766	167.078	1.00	46.90
10	1217	CB	TYR	A	150	31.126	95.863	167.799	1.00	32.05
	1218	CG	TYR	A	150	32.540	95.971	167.323	1.00	33.00
	1219	CD1	TYR	A	150	33.391	96.933	167.837	1.00	32.03
	1220	CE1	TYR	A	150	34.704	97.018	167.419	1.00	59.03
	1221	CD2	TYR	A	150	33.038	95.093	166.369	1.00	75.94
15	1222	CE2	TYR	A	150	34.349	95.169	165.943	1.00	69.80
	1223	CZ	TYR	A	150	35.177	96.135	166.473	1.00	46.28
	1224	OH	TYR	A	150	36.476	96.223	166.049	1.00	71.42
	1225	C	TYR	A	150	30.667	98.182	166.902	1.00	52.29
	1226	O	TYR	A	150	31.175	98.516	165.836	1.00	49.86
20	1227	N	CYS	A	151	30.517	99.025	167.923	1.00	31.32
	1228	CA	CYS	A	151	30.989	100.393	167.832	1.00	7.95
	1229	C	CYS	A	151	31.968	100.769	168.914	1.00	40.57
	1230	O	CYS	A	151	32.057	100.120	169.946	1.00	51.30
	1231	CB	CYS	A	151	29.813	101.372	167.856	1.00	53.04
25	1232	SG	CYS	A	151	28.694	101.368	169.294	1.00	69.58
	1233	N	THR	A	152	32.708	101.835	168.663	1.00	26.38
	1234	CA	THR	A	152	33.671	102.341	169.617	1.00	14.07
	1235	CB	THR	A	152	35.085	102.028	169.185	1.00	22.97
	1236	OG1	THR	A	152	35.335	102.632	167.916	1.00	43.42
30	1237	CG2	THR	A	152	35.276	100.549	169.055	1.00	54.46
	1238	C	THR	A	152	33.489	103.840	169.620	1.00	59.80
	1239	O	THR	A	152	32.993	104.417	168.645	1.00	26.00
	1240	N	GLY	A	153	33.890	104.471	170.715	1.00	24.03
	1241	CA	GLY	A	153	33.751	105.909	170.812	1.00	38.00
35	1242	C	GLY	A	153	34.368	106.444	172.082	1.00	50.23
	1243	O	GLY	A	153	34.734	105.680	172.984	1.00	10.68
	1244	N	LYS	A	154	34.497	107.762	172.155	1.00	20.76
	1245	CA	LYS	A	154	35.071	108.364	173.336	1.00	22.57
	1246	CB	LYS	A	154	36.150	109.375	172.947	1.00	18.43
40	1247	CG	LYS	A	154	37.401	108.744	172.357	1.00	68.32
	1248	CD	LYS	A	154	38.459	109.762	171.955	1.00	79.74
	1249	CE	LYS	A	154	39.759	109.070	171.557	1.00	96.73
	1250	NZ	LYS	A	154	40.839	110.040	171.221	1.00	103.77
	1251	C	LYS	A	154	33.937	109.023	174.095	1.00	49.37
45	1252	O	LYS	A	154	33.075	109.656	173.498	1.00	37.93
	1253	N	VAL	A	155	33.941	108.831	175.411	1.00	29.99
	1254	CA	VAL	A	155	32.935	109.355	176.314	1.00	9.34
	1255	CB	VAL	A	155	32.099	108.223	176.890	1.00	21.29
	1256	CG1	VAL	A	155	31.048	108.748	177.826	1.00	23.90
50	1257	CG2	VAL	A	155	31.476	107.478	175.791	1.00	37.70
	1258	C	VAL	A	155	33.687	109.997	177.457	1.00	27.74
	1259	O	VAL	A	155	34.312	109.306	178.262	1.00	13.56
	1260	N	TRP	A	156	33.627	111.314	177.557	1.00	38.73
	1261	CA	TRP	A	156	34.351	111.977	178.633	1.00	69.64
55	1262	CB	TRP	A	156	33.966	111.410	179.999	1.00	28.52

	1263	CG	TRP	A	156	32.519	111.540	180.386	1.00	64.30
	1264	CD2	TRP	A	156	31.672	112.685	180.244	1.00	16.66
	1265	CE2	TRP	A	156	30.417	112.342	180.786	1.00	65.75
	1266	CE3	TRP	A	156	31.847	113.967	179.715	1.00	72.95
5	1267	CD1	TRP	A	156	31.759	110.583	180.991	1.00	80.53
	1268	NE1	TRP	A	156	30.500	111.052	181.237	1.00	20.03
	1269	CZ2	TRP	A	156	29.348	113.232	180.808	1.00	14.24
	1270	CZ3	TRP	A	156	30.775	114.850	179.744	1.00	11.55
	1271	CH2	TRP	A	156	29.551	114.477	180.284	1.00	40.65
10	1272	C	TRP	A	156	35.834	111.721	178.407	1.00	58.02
	1273	O	TRP	A	156	36.565	111.406	179.334	1.00	32.03
	1274	N	GLN	A	157	36.254	111.828	177.154	1.00	29.52
	1275	CA	GLN	A	157	37.647	111.654	176.770	1.00	71.13
	1276	CB	GLN	A	157	38.515	112.648	177.532	1.00	21.16
15	1277	CG	GLN	A	157	38.719	113.952	176.766	1.00	47.59
	1278	CD	GLN	A	157	38.945	115.134	177.676	1.00	106.91
	1279	OE1	GLN	A	157	39.737	115.068	178.626	1.00	62.17
	1280	NE2	GLN	A	157	38.254	116.237	177.390	1.00	132.54
	1281	C	GLN	A	157	38.273	110.271	176.820	1.00	20.80
20	1282	O	GLN	A	157	39.389	110.086	176.338	1.00	50.51
	1283	N	LEU	A	158	37.569	109.299	177.380	1.00	41.89
	1284	CA	LEU	A	158	38.096	107.940	177.410	1.00	24.44
	1285	CB	LEU	A	158	37.826	107.303	178.761	1.00	29.61
	1286	CG	LEU	A	158	38.450	108.159	179.850	1.00	5.42
25	1287	CD1	LEU	A	158	38.603	107.360	181.127	1.00	45.69
	1288	CD2	LEU	A	158	39.806	108.640	179.378	1.00	68.22
	1289	C	LEU	A	158	37.525	107.073	176.281	1.00	69.39
	1290	O	LEU	A	158	36.521	107.420	175.653	1.00	33.83
	1291	N	ASP	A	159	38.163	105.938	176.024	1.00	33.70
30	1292	CA	ASP	A	159	37.723	105.088	174.933	1.00	15.27
	1293	CB	ASP	A	159	38.940	104.625	174.126	1.00	72.08
	1294	CG	ASP	A	159	39.602	105.757	173.350	1.00	44.73
	1295	OD1	ASP	A	159	38.896	106.450	172.601	1.00	81.88
	1296	OD2	ASP	A	159	40.830	105.951	173.470	1.00	105.33
35	1297	C	ASP	A	159	36.897	103.886	175.355	1.00	50.78
	1298	O	ASP	A	159	37.192	103.224	176.356	1.00	42.36
	1299	N	TYR	A	160	35.859	103.602	174.577	1.00	14.41
	1300	CA	TYR	A	160	35.006	102.466	174.875	1.00	19.18
	1301	CB	TYR	A	160	33.779	102.923	175.654	1.00	30.10
40	1302	CG	TYR	A	160	34.112	103.527	177.002	1.00	39.60
	1303	CD1	TYR	A	160	34.388	104.884	177.140	1.00	9.47
	1304	CE1	TYR	A	160	34.750	105.418	178.371	1.00	50.45
	1305	CD2	TYR	A	160	34.198	102.725	178.131	1.00	36.31
	1306	CE2	TYR	A	160	34.551	103.247	179.361	1.00	31.00
45	1307	CZ	TYR	A	160	34.830	104.587	179.480	1.00	32.81
	1308	OH	TYR	A	160	35.206	105.063	180.718	1.00	38.13
	1309	C	TYR	A	160	34.583	101.703	173.629	1.00	62.53
	1310	O	TYR	A	160	34.549	102.246	172.520	1.00	45.60
	1311	N	GLU	A	161	34.249	100.435	173.824	1.00	46.69
50	1312	CA	GLU	A	161	33.852	99.563	172.727	1.00	47.10
	1313	CB	GLU	A	161	35.018	98.620	172.417	1.00	44.91
	1314	CG	GLU	A	161	34.882	97.745	171.191	1.00	102.74
	1315	CD	GLU	A	161	36.108	96.855	170.973	1.00	98.25
	1316	OE1	GLU	A	161	36.103	96.032	170.030	1.00	115.20
55	1317	OE2	GLU	A	161	37.079	96.980	171.749	1.00	83.84

	1318	C	GLU	A	161	32.617	98.782	173.181	1.00	57.73
	1319	O	GLU	A	161	32.586	98.245	174.284	1.00	75.56
	1320	N	SER	A	162	31.594	98.741	172.337	1.00	36.86
	1321	CA	SER	A	162	30.355	98.038	172.646	1.00	24.23
5	1322	CB	SER	A	162	29.258	98.474	171.679	1.00	85.17
	1323	OG	SER	A	162	29.691	98.382	170.325	1.00	33.98
	1324	C	SER	A	162	30.546	96.549	172.518	1.00	41.42
	1325	O	SER	A	162	31.379	96.108	171.739	1.00	40.06
	1326	N	GLU	A	163	29.828	95.793	173.363	1.00	47.31
10	1327	CA	GLU	A	163	29.945	94.371	173.069	1.00	32.63
	1328	CB	GLU	A	163	29.169	93.547	174.097	1.00	99.44
	1329	CG	GLU	A	163	29.649	93.729	175.527	1.00	204.45
	1330	CD	GLU	A	163	28.850	92.906	176.519	1.00	213.27
	1331	OE1	GLU	A	163	27.925	92.187	176.086	1.00	189.41
15	1332	OE2	GLU	A	163	29.148	92.980	177.729	1.00	180.03
	1333	C	GLU	A	163	29.462	94.059	171.657	1.00	38.80
	1334	O	GLU	A	163	28.601	94.902	171.253	1.00	51.57
	1335	N	PRO	A	164	30.006	93.173	170.942	1.00	52.67
	1336	CD	PRO	A	164	30.968	92.184	171.457	1.00	85.33
20	1337	CA	PRO	A	164	29.650	92.869	169.551	1.00	18.17
	1338	CB	PRO	A	164	30.698	91.847	169.156	1.00	48.35
	1339	CG	PRO	A	164	30.886	91.089	170.416	1.00	83.53
	1340	C	PRO	A	164	28.238	92.378	169.300	1.00	33.91
	1341	O	PRO	A	164	27.605	91.799	170.180	1.00	41.04
25	1342	N	LEU	A	165	27.760	92.592	168.077	1.00	50.63
	1343	CA	LEU	A	165	26.402	92.200	167.706	1.00	22.85
	1344	CB	LEU	A	165	25.483	93.404	167.777	1.00	65.50
	1345	CG	LEU	A	165	24.027	93.057	167.530	1.00	5.42
	1346	CD1	LEU	A	165	23.591	92.064	168.578	1.00	85.48
30	1347	CD2	LEU	A	165	23.182	94.310	167.584	1.00	73.11
	1348	C	LEU	A	165	26.254	91.591	166.323	1.00	58.98
	1349	O	LEU	A	165	26.696	92.171	165.326	1.00	45.85
	1350	N	ASN	A	166	25.586	90.441	166.269	1.00	60.58
	1351	CA	ASN	A	166	25.362	89.731	165.018	1.00	45.14
35	1352	CB	ASN	A	166	25.362	88.226	165.258	1.00	79.77
	1353	CG	ASN	A	166	26.748	87.681	165.468	1.00	84.12
	1354	OD1	ASN	A	166	27.672	88.071	164.756	1.00	37.27
	1355	ND2	ASN	A	166	26.900	86.775	166.428	1.00	83.10
	1356	C	ASN	A	166	24.079	90.124	164.312	1.00	53.27
40	1357	O	ASN	A	166	23.018	90.241	164.919	1.00	65.38
	1358	N	ILE	A	167	24.195	90.314	163.008	1.00	52.39
	1359	CA	ILE	A	167	23.071	90.689	162.171	1.00	51.60
	1360	CB	ILE	A	167	23.197	92.152	161.735	1.00	54.96
	1361	CG2	ILE	A	167	22.259	92.454	160.598	1.00	34.47
45	1362	CG1	ILE	A	167	22.875	93.055	162.912	1.00	29.93
	1363	CD1	ILE	A	167	23.061	94.512	162.595	1.00	110.11
	1364	C	ILE	A	167	23.023	89.784	160.944	1.00	77.50
	1365	O	ILE	A	167	24.024	89.605	160.245	1.00	94.63
	1366	N	THR	A	168	21.844	89.226	160.691	1.00	79.37
50	1367	CA	THR	A	168	21.635	88.318	159.573	1.00	66.36
	1368	CB	THR	A	168	21.250	86.945	160.109	1.00	55.12
	1369	OG1	THR	A	168	20.149	87.094	161.014	1.00	103.78
	1370	CG2	THR	A	168	22.416	86.313	160.856	1.00	86.09
	1371	C	THR	A	168	20.545	88.797	158.607	1.00	74.59
55	1372	O	THR	A	168	19.565	89.412	159.024	1.00	64.58

	1373	N	VAL	A	169	20.718	88.502	157.320	1.00	76.13
	1374	CA	VAL	A	169	19.752	88.894	156.291	1.00	70.39
	1375	CB	VAL	A	169	20.320	90.056	155.456	1.00	62.07
	1376	CG1	VAL	A	169	19.381	90.419	154.335	1.00	100.15
5	1377	CG2	VAL	A	169	20.529	91.251	156.341	1.00	62.65
	1378	C	VAL	A	169	19.382	87.703	155.386	1.00	94.90
	1379	O	VAL	A	169	20.259	86.968	154.931	1.00	115.53
	1380	N	ILE	A	170	18.081	87.537	155.123	1.00	88.61
	1381	CA	ILE	A	170	17.538	86.422	154.329	1.00	131.29
10	1382	CB	ILE	A	170	16.224	85.933	154.969	1.00	132.04
	1383	CG2	ILE	A	170	15.908	84.511	154.513	1.00	178.52
	1384	CG1	ILE	A	170	16.360	85.966	156.492	1.00	77.40
	1385	CD1	ILE	A	170	15.077	85.661	157.225	1.00	74.21
	1386	C	ILE	A	170	17.264	86.673	152.835	1.00	163.13
15	1387	O	ILE	A	170	17.487	87.768	152.330	1.00	191.77
	1388	N	LYS	A	171	16.781	85.637	152.142	1.00	174.37
	1389	CA	LYS	A	171	16.446	85.699	150.713	1.00	184.81
	1390	CB	LYS	A	171	17.572	85.098	149.861	1.00	169.16
	1391	CG	LYS	A	171	18.821	85.950	149.771	1.00	171.69
20	1392	CD	LYS	A	171	19.841	85.352	148.814	1.00	165.73
	1393	CE	LYS	A	171	21.059	86.259	148.692	1.00	166.52
	1394	NZ	LYS	A	171	22.110	85.721	147.784	1.00	163.94
	1395	C	LYS	A	171	15.152	84.928	150.430	1.00	199.02
	1396	O	LYS	A	171	14.841	83.961	151.124	1.00	217.89
25	1397	N	ALA	A	172	14.405	85.349	149.410	1.00	194.74
	1398	CA	ALA	A	172	13.152	84.681	149.047	1.00	171.94
	1399	CB	ALA	A	172	11.960	85.501	149.535	1.00	113.16
	1400	C	ALA	A	172	13.055	84.474	147.535	1.00	174.40
	1401	O	ALA	A	172	12.810	85.420	146.788	1.00	182.27
30	1402	N	PRO	A	173	13.241	83.227	147.067	1.00	195.13
	1403	CD	PRO	A	173	13.548	82.010	147.842	1.00	150.42
	1404	CA	PRO	A	173	13.170	82.925	145.632	1.00	196.30
	1405	CB	PRO	A	173	13.702	81.495	145.558	1.00	174.85
	1406	CG	PRO	A	173	13.235	80.907	146.852	1.00	159.72
35	1407	C	PRO	A	173	11.765	83.064	145.034	1.00	184.97
	1408	O	PRO	A	173	11.238	82.054	144.522	1.00	174.19
	1409	OXT	PRO	A	173	11.213	84.183	145.089	1.00	91.11
	1410	C1	NAG	A	221	11.009	106.713	181.607	1.00	78.57
	1411	C2	NAG	A	221	11.997	107.878	181.655	1.00	100.89
40	1412	N2	NAG	A	221	13.311	107.471	181.201	1.00	76.21
	1413	C7	NAG	A	221	13.976	108.256	180.361	1.00	117.38
	1414	O7	NAG	A	221	13.803	108.231	179.142	1.00	148.10
	1415	C8	NAG	A	221	14.971	109.233	180.966	1.00	135.41
	1416	C3	NAG	A	221	12.062	108.405	183.087	1.00	127.09
45	1417	O3	NAG	A	221	12.916	109.541	183.151	1.00	152.40
	1418	C4	NAG	A	221	10.653	108.784	183.562	1.00	126.14
	1419	O4	NAG	A	221	10.688	109.080	184.970	1.00	148.94
	1420	C5	NAG	A	221	9.653	107.645	183.321	1.00	133.04
	1421	O5	NAG	A	221	9.707	107.189	181.953	1.00	70.49
50	1422	C6	NAG	A	221	8.220	108.040	183.621	1.00	149.52
	1423	O6	NAG	A	221	7.694	108.868	182.567	1.00	151.09
	1424	C1	NAG	A	222	10.235	110.337	185.310	1.00	150.76
	1425	C2	NAG	A	222	9.719	110.337	186.759	1.00	157.88
	1426	N2	NAG	A	222	8.580	109.445	186.884	1.00	152.33
55	1427	C7	NAG	A	222	8.427	108.704	187.977	1.00	149.05

	1428	O7	NAG	A	222	9.078	107.677	188.190	1.00	108.16
	1429	C8	NAG	A	222	7.395	109.174	188.991	1.00	148.72
	1430	C3	NAG	A	222	9.316	111.762	187.139	1.00	163.52
	1431	O3	NAG	A	222	8.887	111.804	188.493	1.00	159.10
5	1432	C4	NAG	A	222	10.521	112.683	186.929	1.00	168.36
	1433	O4	NAG	A	222	10.184	114.036	187.276	1.00	195.32
	1434	C5	NAG	A	222	10.970	112.600	185.466	1.00	142.19
	1435	O5	NAG	A	222	11.333	111.244	185.156	1.00	131.31
	1436	C6	NAG	A	222	12.167	113.462	185.127	1.00	147.99
10	1437	O6	NAG	A	222	12.730	113.081	183.879	1.00	139.76
	1438	C1	MAN	A	223	10.805	114.503	188.420	1.00	185.67
	1439	C2	MAN	A	223	10.910	116.025	188.373	1.00	183.28
	1440	O2	MAN	A	223	9.623	116.596	188.179	1.00	182.05
	1441	C3	MAN	A	223	11.524	116.542	189.677	1.00	206.08
15	1442	O3	MAN	A	223	11.463	117.961	189.691	1.00	200.83
	1443	C4	MAN	A	223	10.787	115.976	190.907	1.00	228.59
	1444	O4	MAN	A	223	11.500	116.305	192.093	1.00	213.28
	1445	C5	MAN	A	223	10.646	114.450	190.805	1.00	211.66
	1446	O5	MAN	A	223	10.026	114.090	189.551	1.00	206.15
20	1447	C6	MAN	A	223	9.793	113.860	191.919	1.00	191.52
	1448	O6	MAN	A	223	8.598	113.277	191.412	1.00	161.92
	1449	C1	FUC	A	224	7.359	110.170	182.978	1.00	147.50
	1450	C2	FUC	A	224	6.361	110.756	181.982	1.00	163.07
	1451	O2	FUC	A	224	6.901	110.689	180.670	1.00	142.50
25	1452	C3	FUC	A	224	5.059	109.950	182.059	1.00	147.28
	1453	O3	FUC	A	224	4.101	110.474	181.149	1.00	122.66
	1454	C4	FUC	A	224	4.509	109.992	183.492	1.00	181.93
	1455	O4	FUC	A	224	4.136	111.323	183.829	1.00	194.01
	1456	C5	FUC	A	224	5.573	109.491	184.480	1.00	172.04
30	1457	O5	FUC	A	224	6.810	110.224	184.301	1.00	162.84
	1458	C6	FUC	A	224	5.158	109.661	185.932	1.00	120.33
	1459	C1	NAG	A	242	13.815	85.747	181.704	1.00	57.19
	1460	C2	NAG	A	242	13.676	86.167	183.149	1.00	45.95
	1461	N2	NAG	A	242	12.332	86.630	183.415	1.00	15.33
35	1462	C7	NAG	A	242	11.817	86.468	184.631	1.00	112.91
	1463	O7	NAG	A	242	11.620	85.356	185.127	1.00	100.48
	1464	C8	NAG	A	242	11.482	87.721	185.427	1.00	16.99
	1465	C3	NAG	A	242	14.703	87.257	183.411	1.00	60.32
	1466	O3	NAG	A	242	14.623	87.699	184.764	1.00	42.86
40	1467	C4	NAG	A	242	16.114	86.722	183.109	1.00	61.08
	1468	O4	NAG	A	242	17.042	87.825	183.150	1.00	83.57
	1469	C5	NAG	A	242	16.181	86.065	181.715	1.00	41.47
	1470	O5	NAG	A	242	15.096	85.134	181.520	1.00	54.87
	1471	C6	NAG	A	242	17.467	85.288	181.499	1.00	119.52
45	1472	O6	NAG	A	242	17.381	83.969	182.022	1.00	140.01
	1473	C1	NAG	A	243	18.183	87.704	183.928	1.00	81.48
	1474	C2	NAG	A	243	19.362	88.235	183.120	1.00	38.25
	1475	N2	NAG	A	243	19.591	87.363	181.993	1.00	69.21
	1476	C7	NAG	A	243	19.577	87.863	180.768	1.00	66.57
50	1477	O7	NAG	A	243	19.393	89.057	180.540	1.00	94.86
	1478	C8	NAG	A	243	19.805	86.892	179.623	1.00	48.41
	1479	C3	NAG	A	243	20.625	88.312	183.964	1.00	87.22
	1480	O3	NAG	A	243	21.674	88.894	183.208	1.00	98.62
	1481	C4	NAG	A	243	20.364	89.143	185.212	1.00	76.30
55	1482	O4	NAG	A	243	21.549	89.126	186.040	1.00	94.39

	1483	C5	NAG	A	243	19.170	88.509	185.959	1.00	102.39
	1484	O5	NAG	A	243	17.998	88.494	185.115	1.00	49.63
	1485	C6	NAG	A	243	18.782	89.210	187.244	1.00	122.15
	1486	O6	NAG	A	243	17.997	88.358	188.067	1.00	105.32
5	1487	C1	MAN	A	244	22.078	90.350	186.412	1.00	64.85
	1488	C2	MAN	A	244	22.728	90.214	187.783	1.00	116.22
	1489	O2	MAN	A	244	23.684	89.161	187.744	1.00	77.96
	1490	C3	MAN	A	244	23.402	91.540	188.186	1.00	112.21
	1491	O3	MAN	A	244	24.150	91.370	189.413	1.00	152.31
10	1492	C4	MAN	A	244	24.351	92.024	187.075	1.00	144.57
	1493	O4	MAN	A	244	24.813	93.333	187.385	1.00	193.98
	1494	C5	MAN	A	244	23.633	92.031	185.713	1.00	57.60
	1495	O5	MAN	A	244	23.067	90.728	185.441	1.00	80.63
	1496	C6	MAN	A	244	24.504	92.436	184.513	1.00	53.28
15	1497	O6	MAN	A	244	25.641	91.560	184.352	1.00	64.48
	1498	C1	MAN	A	245	23.427	91.459	190.614	1.00	134.73
	1499	C2	MAN	A	245	24.400	91.435	191.803	1.00	145.85
	1500	O2	MAN	A	245	23.715	91.778	193.000	1.00	115.81
	1501	C3	MAN	A	245	25.063	90.050	191.951	1.00	134.74
20	1502	O3	MAN	A	245	25.754	89.986	193.192	1.00	105.27
	1503	C4	MAN	A	245	24.043	88.898	191.885	1.00	133.62
	1504	O4	MAN	A	245	24.736	87.669	191.714	1.00	67.76
	1505	C5	MAN	A	245	23.061	89.079	190.719	1.00	165.40
	1506	O5	MAN	A	245	22.479	90.403	190.751	1.00	164.09
25	1507	C6	MAN	A	245	21.918	88.081	190.747	1.00	136.99
	1508	O6	MAN	A	245	20.800	88.600	191.453	1.00	163.94
	1509	C1	MAN	A	246	26.745	92.247	183.813	1.00	91.80
	1510	C2	MAN	A	246	27.492	91.359	182.813	1.00	89.53
	1511	O2	MAN	A	246	28.434	92.147	182.107	1.00	75.32
30	1512	C3	MAN	A	246	28.223	90.227	183.536	1.00	97.98
	1513	O3	MAN	A	246	28.995	89.485	182.603	1.00	123.68
	1514	C4	MAN	A	246	29.139	90.790	184.628	1.00	99.73
	1515	O4	MAN	A	246	29.701	89.712	185.368	1.00	70.44
	1516	C5	MAN	A	246	28.338	91.709	185.566	1.00	111.67
35	1517	O5	MAN	A	246	27.651	92.738	184.808	1.00	73.91
	1518	C6	MAN	A	246	29.187	92.408	186.620	1.00	133.93
	1519	O6	MAN	A	246	30.118	93.314	186.037	1.00	157.23
	1520	C1	NAG	A	366	28.056	85.901	166.422	1.00	118.02
	1521	C2	NAG	A	366	27.711	84.597	167.109	1.00	144.13
40	1522	N2	NAG	A	366	27.168	84.844	168.429	1.00	145.90
	1523	C7	NAG	A	366	26.706	83.827	169.147	1.00	187.35
	1524	O7	NAG	A	366	27.404	83.211	169.952	1.00	194.87
	1525	C8	NAG	A	366	25.255	83.418	168.931	1.00	170.13
	1526	C3	NAG	A	366	28.966	83.736	167.196	1.00	142.04
45	1527	O3	NAG	A	366	28.630	82.485	167.776	1.00	194.55
	1528	C4	NAG	A	366	29.556	83.514	165.790	1.00	143.64
	1529	O4	NAG	A	366	30.849	82.871	165.890	1.00	198.08
	1530	C5	NAG	A	366	29.712	84.852	165.035	1.00	84.06
	1531	O5	NAG	A	366	28.487	85.621	165.083	1.00	133.37
50	1532	C6	NAG	A	366	30.057	84.664	163.560	1.00	113.91
	1533	O6	NAG	A	366	29.035	83.880	162.905	1.00	159.48
	1534	C1	NAG	A	367	30.856	81.509	166.161	1.00	189.45
	1535	C2	NAG	A	367	32.125	80.858	165.606	1.00	164.69
	1536	N2	NAG	A	367	32.162	81.012	164.163	1.00	194.38
55	1537	C7	NAG	A	367	33.110	81.749	163.590	1.00	201.09

	1538	O7	NAG	A	367	33.517	82.807	164.072	1.00	175.40
	1539	C8	NAG	A	367	33.703	81.229	162.288	1.00	186.30
	1540	C3	NAG	A	367	32.134	79.368	165.981	1.00	171.43
	1541	O3	NAG	A	367	33.372	78.785	165.603	1.00	182.11
5	1542	C4	NAG	A	367	31.925	79.180	167.489	1.00	181.87
	1543	O4	NAG	A	367	31.768	77.799	167.780	1.00	183.58
	1544	C5	NAG	A	367	30.683	79.946	167.949	1.00	186.74
	1545	O5	NAG	A	367	30.802	81.334	167.581	1.00	198.91
	1546	C6	NAG	A	367	30.463	79.898	169.448	1.00	186.99
10	1547	O6	NAG	A	367	29.081	79.771	169.756	1.00	172.34
	1548	C1	FUC	A	369	29.475	83.367	161.677	1.00	178.37
	1549	C2	FUC	A	369	28.873	81.974	161.447	1.00	178.90
	1550	O2	FUC	A	369	29.095	81.158	162.587	1.00	137.53
	1551	C3	FUC	A	369	27.373	82.084	161.176	1.00	178.26
15	1552	O3	FUC	A	369	26.837	80.797	160.906	1.00	126.18
	1553	C4	FUC	A	369	27.145	83.010	159.982	1.00	193.60
	1554	O4	FUC	A	369	27.752	82.452	158.825	1.00	190.82
	1555	C5	FUC	A	369	27.765	84.381	160.283	1.00	182.89
	1556	O5	FUC	A	369	29.175	84.233	160.576	1.00	193.18
20	1557	C6	FUC	A	369	27.641	85.357	159.126	1.00	137.51
	1558	CB	PRO	B	328	44.233	128.245	175.766	1.00	170.67
	1559	CG	PRO	B	328	43.202	128.349	176.889	1.00	177.05
	1560	C	PRO	B	328	43.060	126.964	173.946	1.00	208.41
	1561	O	PRO	B	328	43.981	126.261	173.518	1.00	173.87
25	1562	N	PRO	B	328	42.116	129.063	174.936	1.00	199.93
	1563	CD	PRO	B	328	42.170	129.366	176.377	1.00	189.57
	1564	CA	PRO	B	328	43.348	128.347	174.529	1.00	198.40
	1565	N	CYS	B	329	41.785	126.575	173.931	1.00	223.49
	1566	CA	CYS	B	329	41.399	125.277	173.386	1.00	213.48
30	1567	C	CYS	B	329	40.595	125.390	172.094	1.00	210.28
	1568	O	CYS	B	329	39.925	124.441	171.686	1.00	203.81
	1569	CB	CYS	B	329	40.596	124.462	174.402	1.00	202.41
	1570	SG	CYS	B	329	40.352	122.737	173.856	1.00	228.51
	1571	N	ASP	B	330	40.647	126.557	171.461	1.00	211.89
35	1572	CA	ASP	B	330	39.960	126.766	170.189	1.00	192.96
	1573	CB	ASP	B	330	39.714	128.266	169.964	1.00	206.60
	1574	CG	ASP	B	330	38.919	128.560	168.691	1.00	207.78
	1575	OD1	ASP	B	330	39.428	128.310	167.577	1.00	198.18
	1576	OD2	ASP	B	330	37.778	129.052	168.806	1.00	197.14
40	1577	C	ASP	B	330	40.978	126.228	169.184	1.00	177.46
	1578	O	ASP	B	330	41.198	126.802	168.117	1.00	190.87
	1579	N	SER	B	331	41.601	125.110	169.550	1.00	151.57
	1580	CA	SER	B	331	42.636	124.492	168.731	1.00	109.39
	1581	CB	SER	B	331	43.959	124.493	169.509	1.00	109.57
45	1582	OG	SER	B	331	43.867	123.728	170.706	1.00	75.56
	1583	C	SER	B	331	42.353	123.073	168.245	1.00	79.09
	1584	O	SER	B	331	43.245	122.411	167.724	1.00	130.44
	1585	N	ASN	B	332	41.129	122.596	168.411	1.00	76.72
	1586	CA	ASN	B	332	40.796	121.246	167.977	1.00	39.06
50	1587	CB	ASN	B	332	40.842	120.285	169.162	1.00	93.86
	1588	CG	ASN	B	332	42.247	119.821	169.484	1.00	76.70
	1589	OD1	ASN	B	332	43.185	120.617	169.523	1.00	81.95
	1590	ND2	ASN	B	332	42.398	118.525	169.735	1.00	60.32
	1591	C	ASN	B	332	39.424	121.189	167.336	1.00	50.77
55	1592	O	ASN	B	332	38.588	120.357	167.696	1.00	48.39

	1593	N	PRO	B	333	39.173	122.079	166.373	1.00	10.22
	1594	CD	PRO	B	333	40.098	123.063	165.794	1.00	26.58
	1595	CA	PRO	B	333	37.889	122.113	165.689	1.00	43.44
	1596	CB	PRO	B	333	38.232	122.764	164.362	1.00	11.09
5	1597	CG	PRO	B	333	39.219	123.787	164.780	1.00	73.63
	1598	C	PRO	B	333	37.271	120.738	165.530	1.00	11.84
	1599	O	PRO	B	333	37.932	119.767	165.206	1.00	62.32
	1600	N	ARG	B	334	35.984	120.677	165.788	1.00	33.64
	1601	CA	ARG	B	334	35.235	119.460	165.677	1.00	33.31
10	1602	CB	ARG	B	334	34.754	119.322	164.242	1.00	10.21
	1603	CG	ARG	B	334	33.904	118.112	164.022	1.00	52.28
	1604	CD	ARG	B	334	32.439	118.403	163.975	1.00	10.85
	1605	NE	ARG	B	334	31.983	118.450	162.597	1.00	39.50
	1606	CZ	ARG	B	334	30.763	118.103	162.210	1.00	75.73
15	1607	NH1	ARG	B	334	29.885	117.676	163.099	1.00	59.45
	1608	NH2	ARG	B	334	30.416	118.202	160.936	1.00	61.90
	1609	C	ARG	B	334	36.002	118.225	166.156	1.00	35.54
	1610	O	ARG	B	334	35.615	117.090	165.891	1.00	57.63
	1611	N	GLY	B	335	37.081	118.441	166.896	1.00	21.32
20	1612	CA	GLY	B	335	37.832	117.308	167.413	1.00	60.66
	1613	C	GLY	B	335	39.060	116.972	166.600	1.00	46.23
	1614	O	GLY	B	335	39.953	116.256	167.053	1.00	28.43
	1615	N	VAL	B	336	39.087	117.491	165.381	1.00	51.37
	1616	CA	VAL	B	336	40.196	117.306	164.454	1.00	36.83
25	1617	CB	VAL	B	336	39.836	117.952	163.124	1.00	62.63
	1618	CG1	VAL	B	336	41.025	117.972	162.204	1.00	75.33
	1619	CG2	VAL	B	336	38.674	117.213	162.512	1.00	96.26
	1620	C	VAL	B	336	41.485	117.947	164.969	1.00	35.62
	1621	O	VAL	B	336	41.596	119.164	164.967	1.00	59.08
30	1622	N	SER	B	337	42.456	117.148	165.404	1.00	44.91
	1623	CA	SER	B	337	43.714	117.712	165.900	1.00	35.01
	1624	CB	SER	B	337	44.232	116.895	167.081	1.00	70.32
	1625	OG	SER	B	337	44.222	115.512	166.795	1.00	72.41
	1626	C	SER	B	337	44.791	117.806	164.809	1.00	48.70
35	1627	O	SER	B	337	44.673	117.177	163.760	1.00	25.48
	1628	N	ALA	B	338	45.827	118.612	165.058	1.00	48.51
	1629	CA	ALA	B	338	46.939	118.821	164.107	1.00	82.57
	1630	CB	ALA	B	338	46.705	120.063	163.245	1.00	7.76
	1631	C	ALA	B	338	48.260	118.980	164.842	1.00	29.51
40	1632	O	ALA	B	338	48.301	119.477	165.968	1.00	84.58
	1633	N	TYR	B	339	49.340	118.555	164.206	1.00	63.43
	1634	CA	TYR	B	339	50.643	118.655	164.823	1.00	60.91
	1635	CB	TYR	B	339	51.122	117.269	165.235	1.00	46.03
	1636	CG	TYR	B	339	50.150	116.534	166.132	1.00	43.69
45	1637	CD1	TYR	B	339	49.014	115.921	165.614	1.00	74.02
	1638	CE1	TYR	B	339	48.098	115.288	166.440	1.00	48.18
	1639	CD2	TYR	B	339	50.347	116.492	167.503	1.00	70.23
	1640	CE2	TYR	B	339	49.435	115.867	168.340	1.00	97.07
	1641	CZ	TYR	B	339	48.310	115.270	167.804	1.00	86.05
50	1642	OH	TYR	B	339	47.383	114.696	168.648	1.00	102.25
	1643	C	TYR	B	339	51.610	119.290	163.841	1.00	88.66
	1644	O	TYR	B	339	51.530	119.048	162.640	1.00	48.34
	1645	N	LEU	B	340	52.515	120.118	164.348	1.00	69.25
	1646	CA	LEU	B	340	53.476	120.776	163.479	1.00	62.80
55	1647	CB	LEU	B	340	53.186	122.263	163.438	1.00	27.87

	1648	CG	LEU	B	340	54.027	123.160	162.544	1.00	34.78
	1649	CD1	LEU	B	340	53.820	122.802	161.089	1.00	68.67
	1650	CD2	LEU	B	340	53.615	124.594	162.770	1.00	83.17
	1651	C	LEU	B	340	54.881	120.531	163.988	1.00	79.88
5	1652	O	LEU	B	340	55.294	121.133	164.972	1.00	77.02
	1653	N	SER	B	341	55.612	119.651	163.305	1.00	82.92
	1654	CA	SER	B	341	56.964	119.290	163.712	1.00	91.09
	1655	CB	SER	B	341	57.333	117.925	163.139	1.00	105.90
	1656	OG	SER	B	341	58.517	117.431	163.744	1.00	156.83
10	1657	C	SER	B	341	58.023	120.306	163.321	1.00	86.74
	1658	O	SER	B	341	57.918	120.956	162.286	1.00	74.60
	1659	N	ARG	B	342	59.045	120.419	164.168	1.00	108.27
	1660	CA	ARG	B	342	60.165	121.343	163.976	1.00	58.14
	1661	CB	ARG	B	342	60.602	121.890	165.343	1.00	98.53
15	1662	CG	ARG	B	342	60.649	120.808	166.429	1.00	141.70
	1663	CD	ARG	B	342	61.354	121.239	167.726	1.00	145.30
	1664	NE	ARG	B	342	60.568	122.139	168.567	1.00	104.32
	1665	CZ	ARG	B	342	60.430	123.442	168.351	1.00	124.08
	1666	NH1	ARG	B	342	61.028	124.015	167.315	1.00	83.45
20	1667	NH2	ARG	B	342	59.691	124.174	169.173	1.00	139.46
	1668	C	ARG	B	342	61.352	120.635	163.287	1.00	98.70
	1669	O	ARG	B	342	61.582	119.441	163.500	1.00	94.69
	1670	N	PRO	B	343	62.120	121.368	162.457	1.00	62.71
	1671	CD	PRO	B	343	62.016	122.823	162.278	1.00	69.22
25	1672	CA	PRO	B	343	63.281	120.850	161.728	1.00	36.63
	1673	CB	PRO	B	343	63.916	122.104	161.148	1.00	63.75
	1674	CG	PRO	B	343	62.776	123.035	161.003	1.00	46.63
	1675	C	PRO	B	343	64.234	120.174	162.689	1.00	50.31
	1676	O	PRO	B	343	64.518	120.713	163.762	1.00	73.12
30	1677	N	SER	B	344	64.737	119.002	162.311	1.00	83.43
	1678	CA	SER	B	344	65.671	118.289	163.177	1.00	70.61
	1679	CB	SER	B	344	65.778	116.812	162.781	1.00	82.96
	1680	OG	SER	B	344	66.324	116.661	161.483	1.00	84.14
	1681	C	SER	B	344	67.024	118.946	163.041	1.00	65.68
35	1682	O	SER	B	344	67.334	119.517	161.998	1.00	50.07
	1683	N	PRO	B	345	67.844	118.894	164.104	1.00	74.48
	1684	CD	PRO	B	345	67.611	118.184	165.375	1.00	88.87
	1685	CA	PRO	B	345	69.183	119.494	164.081	1.00	69.58
	1686	CB	PRO	B	345	69.862	118.867	165.296	1.00	81.66
40	1687	CG	PRO	B	345	68.745	118.694	166.255	1.00	59.69
	1688	C	PRO	B	345	69.849	119.065	162.789	1.00	83.15
	1689	O	PRO	B	345	70.233	119.893	161.960	1.00	54.26
	1690	N	PHE	B	346	69.955	117.745	162.642	1.00	65.25
	1691	CA	PHE	B	346	70.542	117.099	161.482	1.00	38.65
45	1692	CB	PHE	B	346	70.209	115.611	161.522	1.00	67.61
	1693	CG	PHE	B	346	70.755	114.839	160.365	1.00	96.31
	1694	CD1	PHE	B	346	72.119	114.727	160.181	1.00	76.06
	1695	CD2	PHE	B	346	69.903	114.239	159.445	1.00	132.61
	1696	CE1	PHE	B	346	72.632	114.039	159.104	1.00	96.72
50	1697	CE2	PHE	B	346	70.410	113.544	158.358	1.00	124.94
	1698	CZ	PHE	B	346	71.779	113.445	158.187	1.00	134.65
	1699	C	PHE	B	346	70.045	117.721	160.170	1.00	58.29
	1700	O	PHE	B	346	70.796	118.379	159.474	1.00	57.14
	1701	N	ASP	B	347	68.777	117.524	159.831	1.00	56.88
55	1702	CA	ASP	B	347	68.226	118.078	158.592	1.00	64.19

	1703	CB	ASP	B	347	66.703	117.859	158.542	1.00	98.15
	1704	CG	ASP	B	347	66.318	116.431	158.211	1.00	120.11
	1705	OD1	ASP	B	347	66.506	116.024	157.046	1.00	142.93
	1706	OD2	ASP	B	347	65.826	115.715	159.112	1.00	148.42
5	1707	C	ASP	B	347	68.509	119.576	158.466	1.00	78.62
	1708	O	ASP	B	347	68.339	120.174	157.401	1.00	40.12
	1709	N	LEU	B	348	68.969	120.178	159.550	1.00	43.72
	1710	CA	LEU	B	348	69.184	121.613	159.553	1.00	79.44
	1711	CB	LEU	B	348	68.570	122.183	160.837	1.00	64.43
10	1712	CG	LEU	B	348	68.601	123.691	161.101	1.00	74.91
	1713	CD1	LEU	B	348	68.208	124.482	159.860	1.00	80.89
	1714	CD2	LEU	B	348	67.656	123.985	162.246	1.00	82.45
	1715	C	LEU	B	348	70.617	122.094	159.396	1.00	77.53
	1716	O	LEU	B	348	70.863	123.165	158.841	1.00	66.37
15	1717	N	PHE	B	349	71.560	121.300	159.877	1.00	81.75
	1718	CA	PHE	B	349	72.964	121.666	159.811	1.00	90.94
	1719	CB	PHE	B	349	73.515	121.657	161.221	1.00	89.74
	1720	CG	PHE	B	349	72.864	122.665	162.096	1.00	88.86
	1721	CD1	PHE	B	349	72.745	122.458	163.464	1.00	102.92
20	1722	CD2	PHE	B	349	72.363	123.837	161.542	1.00	48.94
	1723	CE1	PHE	B	349	72.133	123.406	164.274	1.00	64.93
	1724	CE2	PHE	B	349	71.754	124.786	162.335	1.00	94.98
	1725	CZ	PHE	B	349	71.638	124.572	163.708	1.00	102.89
	1726	C	PHE	B	349	73.806	120.800	158.889	1.00	102.94
25	1727	O	PHE	B	349	74.633	121.304	158.137	1.00	120.26
	1728	N	ILE	B	350	73.609	119.494	158.963	1.00	100.45
	1729	CA	ILE	B	350	74.328	118.586	158.098	1.00	57.80
	1730	CB	ILE	B	350	74.145	117.136	158.545	1.00	71.44
	1731	CG2	ILE	B	350	74.830	116.213	157.588	1.00	91.54
30	1732	CG1	ILE	B	350	74.662	116.959	159.972	1.00	71.63
	1733	CD1	ILE	B	350	76.040	117.471	160.193	1.00	65.43
	1734	C	ILE	B	350	73.672	118.752	156.738	1.00	76.53
	1735	O	ILE	B	350	74.101	119.559	155.928	1.00	93.37
	1736	N	ARG	B	351	72.601	117.998	156.520	1.00	76.58
35	1737	CA	ARG	B	351	71.852	118.003	155.261	1.00	85.35
	1738	CB	ARG	B	351	70.544	117.223	155.464	1.00	94.17
	1739	CG	ARG	B	351	69.978	116.539	154.229	1.00	114.26
	1740	CD	ARG	B	351	69.081	115.375	154.644	1.00	134.12
	1741	NE	ARG	B	351	68.530	114.661	153.497	1.00	180.07
40	1742	CZ	ARG	B	351	67.646	115.179	152.650	1.00	196.67
	1743	NH1	ARG	B	351	67.210	116.420	152.821	1.00	201.25
	1744	NH2	ARG	B	351	67.198	114.456	151.632	1.00	193.34
	1745	C	ARG	B	351	71.563	119.406	154.722	1.00	85.97
	1746	O	ARG	B	351	71.257	119.576	153.546	1.00	79.18
45	1747	N	LYS	B	352	71.672	120.401	155.594	1.00	70.30
	1748	CA	LYS	B	352	71.417	121.800	155.249	1.00	116.58
	1749	CB	LYS	B	352	72.641	122.404	154.559	1.00	144.96
	1750	CG	LYS	B	352	73.881	122.501	155.448	1.00	168.84
	1751	CD	LYS	B	352	74.894	123.491	154.874	1.00	186.41
50	1752	CE	LYS	B	352	76.217	123.484	155.633	1.00	172.60
	1753	NZ	LYS	B	352	77.028	122.264	155.354	1.00	186.13
	1754	C	LYS	B	352	70.162	122.102	154.416	1.00	119.94
	1755	O	LYS	B	352	70.110	123.108	153.709	1.00	105.59
	1756	N	SER	B	353	69.160	121.231	154.504	1.00	128.80
55	1757	CA	SER	B	353	67.884	121.411	153.802	1.00	102.46

	1758	CB	SER	B	353	67.788	120.501	152.574	1.00	122.75
	1759	OG	SER	B	353	67.784	119.131	152.936	1.00	168.70
	1760	C	SER	B	353	66.811	121.034	154.818	1.00	99.64
	1761	O	SER	B	353	66.337	119.897	154.860	1.00	93.09
5	1762	N	PRO	B	354	66.421	121.994	155.661	1.00	84.24
	1763	CD	PRO	B	354	66.948	123.357	155.738	1.00	97.02
	1764	CA	PRO	B	354	65.415	121.793	156.698	1.00	77.36
	1765	CB	PRO	B	354	65.720	122.910	157.702	1.00	87.64
	1766	CG	PRO	B	354	67.006	123.540	157.208	1.00	75.30
10	1767	C	PRO	B	354	63.998	121.894	156.181	1.00	95.66
	1768	O	PRO	B	354	63.722	122.632	155.225	1.00	61.77
	1769	N	THR	B	355	63.108	121.145	156.826	1.00	83.51
	1770	CA	THR	B	355	61.696	121.153	156.478	1.00	60.49
	1771	CB	THR	B	355	61.340	120.121	155.405	1.00	59.24
15	1772	OG1	THR	B	355	61.685	118.810	155.876	1.00	77.07
	1773	CG2	THR	B	355	62.053	120.440	154.098	1.00	114.79
	1774	C	THR	B	355	60.837	120.838	157.683	1.00	79.73
	1775	O	THR	B	355	61.132	119.924	158.464	1.00	73.10
	1776	N	ILE	B	356	59.765	121.613	157.815	1.00	73.22
20	1777	CA	ILE	B	356	58.801	121.449	158.891	1.00	76.70
	1778	CB	ILE	B	356	58.351	122.805	159.441	1.00	47.99
	1779	CG2	ILE	B	356	59.496	123.453	160.194	1.00	83.94
	1780	CG1	ILE	B	356	57.861	123.691	158.294	1.00	66.86
	1781	CD1	ILE	B	356	57.478	125.075	158.729	1.00	80.08
25	1782	C	ILE	B	356	57.595	120.723	158.311	1.00	74.21
	1783	O	ILE	B	356	57.290	120.849	157.110	1.00	45.14
	1784	N	THR	B	357	56.898	119.978	159.164	1.00	59.52
	1785	CA	THR	B	357	55.752	119.215	158.706	1.00	66.63
	1786	CB	THR	B	357	56.095	117.748	158.697	1.00	60.44
30	1787	OG1	THR	B	357	57.388	117.574	158.106	1.00	96.24
	1788	CG2	THR	B	357	55.066	116.981	157.904	1.00	78.11
	1789	C	THR	B	357	54.494	119.395	159.534	1.00	65.25
	1790	O	THR	B	357	54.525	119.290	160.762	1.00	62.91
	1791	N	CYS	B	358	53.387	119.639	158.836	1.00	60.07
35	1792	CA	CYS	B	358	52.076	119.835	159.453	1.00	60.41
	1793	C	CYS	B	358	51.260	118.568	159.245	1.00	47.28
	1794	O	CYS	B	358	50.999	118.164	158.117	1.00	61.76
	1795	CB	CYS	B	358	51.372	121.006	158.789	1.00	66.79
	1796	SG	CYS	B	358	49.884	121.601	159.632	1.00	87.73
40	1797	N	LEU	B	359	50.862	117.934	160.334	1.00	55.07
	1798	CA	LEU	B	359	50.102	116.700	160.248	1.00	25.58
	1799	CB	LEU	B	359	50.884	115.602	160.956	1.00	60.22
	1800	CG	LEU	B	359	50.116	114.353	161.371	1.00	17.72
	1801	CD1	LEU	B	359	49.435	113.786	160.175	1.00	49.40
45	1802	CD2	LEU	B	359	51.037	113.345	162.002	1.00	86.18
	1803	C	LEU	B	359	48.703	116.836	160.859	1.00	39.46
	1804	O	LEU	B	359	48.538	117.114	162.044	1.00	57.72
	1805	N	VAL	B	360	47.692	116.631	160.034	1.00	50.02
	1806	CA	VAL	B	360	46.316	116.727	160.476	1.00	35.99
50	1807	CB	VAL	B	360	45.467	117.468	159.452	1.00	46.54
	1808	CG1	VAL	B	360	44.028	117.436	159.862	1.00	47.57
	1809	CG2	VAL	B	360	45.948	118.886	159.328	1.00	29.82
	1810	C	VAL	B	360	45.751	115.334	160.628	1.00	34.08
	1811	O	VAL	B	360	45.885	114.501	159.733	1.00	60.52
55	1812	N	VAL	B	361	45.102	115.091	161.759	1.00	22.24

	1813	CA	VAL	B	361	44.520	113.790	162.040	1.00	37.22
	1814	CB	VAL	B	361	45.305	113.117	163.163	1.00	11.28
	1815	CG1	VAL	B	361	46.626	113.793	163.312	1.00	37.36
	1816	CG2	VAL	B	361	44.563	113.194	164.430	1.00	36.29
5	1817	C	VAL	B	361	43.032	113.828	162.424	1.00	32.87
	1818	O	VAL	B	361	42.504	114.859	162.814	1.00	47.67
	1819	N	ASP	B	362	42.374	112.680	162.324	1.00	50.85
	1820	CA	ASP	B	362	40.963	112.540	162.657	1.00	28.87
	1821	CB	ASP	B	362	40.697	112.967	164.092	1.00	43.13
10	1822	CG	ASP	B	362	41.283	111.999	165.107	1.00	96.71
	1823	OD1	ASP	B	362	41.186	110.772	164.910	1.00	61.11
	1824	OD2	ASP	B	362	41.832	112.464	166.122	1.00	95.29
	1825	C	ASP	B	362	39.978	113.227	161.726	1.00	39.54
	1826	O	ASP	B	362	38.838	113.482	162.112	1.00	44.37
15	1827	N	LEU	B	363	40.410	113.513	160.500	1.00	30.82
	1828	CA	LEU	B	363	39.536	114.118	159.506	1.00	21.83
	1829	CB	LEU	B	363	40.328	114.589	158.298	1.00	31.47
	1830	CG	LEU	B	363	41.130	115.877	158.418	1.00	45.22
	1831	CD1	LEU	B	363	42.030	116.037	157.201	1.00	61.55
20	1832	CD2	LEU	B	363	40.174	117.029	158.514	1.00	33.26
	1833	C	LEU	B	363	38.608	113.026	159.049	1.00	44.60
	1834	O	LEU	B	363	38.922	111.859	159.163	1.00	46.41
	1835	N	ALA	B	364	37.455	113.392	158.533	1.00	51.90
	1836	CA	ALA	B	364	36.541	112.383	158.045	1.00	22.74
25	1837	CB	ALA	B	364	35.186	112.587	158.647	1.00	51.33
	1838	C	ALA	B	364	36.464	112.500	156.530	1.00	60.62
	1839	O	ALA	B	364	36.529	113.603	155.972	1.00	44.38
	1840	N	PRO	B	365	36.339	111.365	155.837	1.00	18.39
	1841	CD	PRO	B	365	35.980	110.033	156.333	1.00	51.04
30	1842	CA	PRO	B	365	36.255	111.404	154.379	1.00	40.07
	1843	CB	PRO	B	365	35.930	109.963	154.027	1.00	109.08
	1844	CG	PRO	B	365	35.117	109.531	155.214	1.00	40.87
	1845	C	PRO	B	365	35.132	112.340	153.965	1.00	58.17
	1846	O	PRO	B	365	34.127	112.428	154.672	1.00	50.80
35	1847	N	SER	B	366	35.303	113.028	152.833	1.00	35.27
	1848	CA	SER	B	366	34.292	113.944	152.315	1.00	93.15
	1849	CB	SER	B	366	34.314	115.271	153.076	1.00	108.06
	1850	OG	SER	B	366	35.515	115.977	152.855	1.00	71.65
	1851	C	SER	B	366	34.515	114.210	150.839	1.00	44.93
40	1852	O	SER	B	366	35.556	113.866	150.290	1.00	106.10
	1853	N	LYS	B	367	33.529	114.827	150.198	1.00	130.17
	1854	CA	LYS	B	367	33.600	115.155	148.779	1.00	79.40
	1855	CB	LYS	B	367	32.319	115.878	148.331	1.00	125.03
	1856	CG	LYS	B	367	31.050	115.020	148.296	1.00	164.89
45	1857	CD	LYS	B	367	29.862	115.815	147.732	1.00	160.83
	1858	CE	LYS	B	367	28.612	114.952	147.548	1.00	137.20
	1859	NZ	LYS	B	367	27.489	115.720	146.924	1.00	126.69
	1860	C	LYS	B	367	34.806	116.040	148.477	1.00	52.10
	1861	O	LYS	B	367	35.562	115.774	147.544	1.00	108.75
50	1862	N	GLY	B	368	34.986	117.089	149.272	1.00	66.48
	1863	CA	GLY	B	368	36.093	117.999	149.043	1.00	81.03
	1864	C	GLY	B	368	37.267	117.768	149.965	1.00	56.47
	1865	O	GLY	B	368	37.106	117.247	151.062	1.00	92.39
	1866	N	THR	B	369	38.455	118.154	149.516	1.00	59.57
55	1867	CA	THR	B	369	39.659	117.986	150.313	1.00	61.18

	1868	CB	THR	B	369	40.891	117.867	149.416	1.00	71.21
	1869	OG1	THR	B	369	41.072	119.088	148.693	1.00	96.74
	1870	CG2	THR	B	369	40.710	116.731	148.420	1.00	106.84
	1871	C	THR	B	369	39.802	119.215	151.181	1.00	47.36
5	1872	O	THR	B	369	39.091	120.193	150.985	1.00	60.95
	1873	N	VAL	B	370	40.712	119.183	152.142	1.00	34.09
	1874	CA	VAL	B	370	40.888	120.349	152.999	1.00	48.60
	1875	CB	VAL	B	370	41.744	120.043	154.219	1.00	24.99
	1876	CG1	VAL	B	370	41.249	118.771	154.883	1.00	36.87
10	1877	CG2	VAL	B	370	43.201	119.920	153.814	1.00	68.00
	1878	C	VAL	B	370	41.552	121.468	152.225	1.00	25.41
	1879	O	VAL	B	370	41.788	121.345	151.027	1.00	88.63
	1880	N	ASN	B	371	41.866	122.554	152.915	1.00	53.72
	1881	CA	ASN	B	371	42.477	123.715	152.290	1.00	52.65
15	1882	CB	ASN	B	371	41.401	124.794	152.091	1.00	74.57
	1883	CG	ASN	B	371	41.906	126.001	151.353	1.00	115.17
	1884	OD1	ASN	B	371	43.097	126.127	151.082	1.00	164.46
	1885	ND2	ASN	B	371	40.996	126.917	151.034	1.00	174.36
	1886	C	ASN	B	371	43.581	124.172	153.235	1.00	58.62
20	1887	O	ASN	B	371	43.409	125.079	154.042	1.00	79.32
	1888	N	LEU	B	372	44.713	123.489	153.130	1.00	85.89
	1889	CA	LEU	B	372	45.903	123.722	153.936	1.00	45.57
	1890	CB	LEU	B	372	46.816	122.511	153.816	1.00	37.74
	1891	CG	LEU	B	372	47.914	122.228	154.841	1.00	36.14
25	1892	CD1	LEU	B	372	48.335	123.493	155.586	1.00	42.25
	1893	CD2	LEU	B	372	47.373	121.176	155.809	1.00	26.23
	1894	C	LEU	B	372	46.605	124.937	153.369	1.00	69.02
	1895	O	LEU	B	372	46.702	125.071	152.155	1.00	96.74
	1896	N	THR	B	373	47.102	125.818	154.228	1.00	57.25
30	1897	CA	THR	B	373	47.760	127.025	153.748	1.00	31.14
	1898	CB	THR	B	373	46.741	128.177	153.665	1.00	67.35
	1899	OG1	THR	B	373	45.708	127.832	152.735	1.00	72.32
	1900	CG2	THR	B	373	47.397	129.452	153.211	1.00	83.78
	1901	C	THR	B	373	48.927	127.440	154.633	1.00	76.56
35	1902	O	THR	B	373	48.768	127.635	155.846	1.00	63.76
	1903	N	TRP	B	374	50.099	127.578	154.010	1.00	81.63
	1904	CA	TRP	B	374	51.325	127.962	154.715	1.00	63.39
	1905	CB	TRP	B	374	52.533	127.246	154.128	1.00	60.06
	1906	CG	TRP	B	374	52.577	125.801	154.393	1.00	38.27
40	1907	CD2	TRP	B	374	53.047	125.173	155.583	1.00	17.81
	1908	CE2	TRP	B	374	52.925	123.781	155.398	1.00	26.57
	1909	CE3	TRP	B	374	53.563	125.650	156.784	1.00	45.86
	1910	CD1	TRP	B	374	52.195	124.796	153.549	1.00	58.25
	1911	NE1	TRP	B	374	52.403	123.575	154.149	1.00	41.78
45	1912	CZ2	TRP	B	374	53.300	122.866	156.373	1.00	46.60
	1913	CZ3	TRP	B	374	53.940	124.734	157.759	1.00	44.09
	1914	CH2	TRP	B	374	53.804	123.364	157.548	1.00	18.32
	1915	C	TRP	B	374	51.591	129.457	154.649	1.00	94.67
	1916	O	TRP	B	374	51.341	130.096	153.622	1.00	70.49
50	1917	N	SER	B	375	52.133	130.003	155.735	1.00	79.04
	1918	CA	SER	B	375	52.421	131.428	155.798	1.00	76.64
	1919	CB	SER	B	375	51.136	132.190	156.128	1.00	121.29
	1920	OG	SER	B	375	50.563	131.725	157.343	1.00	115.00
	1921	C	SER	B	375	53.500	131.793	156.818	1.00	100.83
55	1922	O	SER	B	375	53.681	131.114	157.844	1.00	45.77

	1923	N	ARG	B	376	54.215	132.876	156.526	1.00	84.64
	1924	CA	ARG	B	376	55.263	133.366	157.418	1.00	89.30
	1925	CB	ARG	B	376	56.525	133.715	156.631	1.00	108.51
	1926	CG	ARG	B	376	57.394	132.526	156.294	1.00	125.68
5	1927	CD	ARG	B	376	58.852	132.940	156.133	1.00	127.76
	1928	NE	ARG	B	376	59.165	133.476	154.812	1.00	88.17
	1929	CZ	ARG	B	376	60.372	133.898	154.461	1.00	124.32
	1930	NH1	ARG	B	376	61.368	133.849	155.337	1.00	105.92
	1931	NH2	ARG	B	376	60.588	134.349	153.234	1.00	164.32
10	1932	C	ARG	B	376	54.795	134.607	158.167	1.00	120.27
	1933	O	ARG	B	376	53.953	135.367	157.674	1.00	114.07
	1934	N	ALA	B	377	55.344	134.817	159.357	1.00	101.03
	1935	CA	ALA	B	377	54.973	135.981	160.151	1.00	108.48
	1936	CB	ALA	B	377	55.394	135.784	161.583	1.00	88.56
15	1937	C	ALA	B	377	55.607	137.252	159.593	1.00	112.40
	1938	O	ALA	B	377	55.071	138.345	159.751	1.00	124.37
	1939	N	SER	B	378	56.753	137.105	158.943	1.00	101.18
	1940	CA	SER	B	378	57.445	138.242	158.362	1.00	69.51
	1941	CB	SER	B	378	58.845	137.831	157.902	1.00	111.91
20	1942	OG	SER	B	378	58.778	137.003	156.747	1.00	103.91
	1943	C	SER	B	378	56.665	138.786	157.166	1.00	87.46
	1944	O	SER	B	378	56.842	139.936	156.769	1.00	118.01
	1945	N	GLY	B	379	55.807	137.957	156.588	1.00	90.70
	1946	CA	GLY	B	379	55.031	138.392	155.441	1.00	104.68
25	1947	C	GLY	B	379	55.679	137.954	154.143	1.00	122.51
	1948	O	GLY	B	379	55.045	137.946	153.084	1.00	110.08
	1949	N	LYS	B	380	56.950	137.579	154.229	1.00	122.20
	1950	CA	LYS	B	380	57.699	137.136	153.061	1.00	147.83
	1951	CB	LYS	B	380	59.174	136.966	153.428	1.00	162.29
30	1952	CG	LYS	B	380	59.830	138.223	153.989	1.00	173.82
	1953	CD	LYS	B	380	61.286	137.969	154.360	1.00	180.37
	1954	CE	LYS	B	380	61.949	139.218	154.922	1.00	172.23
	1955	NZ	LYS	B	380	63.378	138.976	155.269	1.00	155.65
	1956	C	LYS	B	380	57.145	135.820	152.513	1.00	146.60
35	1957	O	LYS	B	380	56.856	134.897	153.270	1.00	157.16
	1958	N	PRO	B	381	56.992	135.724	151.182	1.00	140.30
	1959	CD	PRO	B	381	57.285	136.796	150.216	1.00	154.76
	1960	CA	PRO	B	381	56.475	134.537	150.493	1.00	131.70
	1961	CB	PRO	B	381	56.787	134.838	149.034	1.00	142.42
40	1962	CG	PRO	B	381	56.572	136.313	148.971	1.00	139.64
	1963	C	PRO	B	381	57.085	133.216	150.966	1.00	119.70
	1964	O	PRO	B	381	58.115	133.207	151.647	1.00	96.93
	1965	N	VAL	B	382	56.443	132.109	150.589	1.00	110.70
	1966	CA	VAL	B	382	56.885	130.765	150.975	1.00	88.04
45	1967	CB	VAL	B	382	55.908	130.140	151.964	1.00	67.75
	1968	CG1	VAL	B	382	55.938	130.895	153.273	1.00	128.08
	1969	CG2	VAL	B	382	54.511	130.160	151.360	1.00	82.52
	1970	C	VAL	B	382	57.020	129.784	149.808	1.00	109.58
	1971	O	VAL	B	382	56.279	129.858	148.817	1.00	109.44
50	1972	N	ASN	B	383	57.958	128.849	149.947	1.00	109.75
	1973	CA	ASN	B	383	58.197	127.845	148.918	1.00	128.69
	1974	CB	ASN	B	383	59.393	126.966	149.309	1.00	135.40
	1975	CG	ASN	B	383	60.723	127.696	149.189	1.00	146.65
	1976	OD1	ASN	B	383	61.759	127.196	149.629	1.00	133.04
55	1977	ND2	ASN	B	383	60.702	128.877	148.582	1.00	137.22

	1978	C	ASN	B	383	56.955	126.981	148.730	1.00	91.22
	1979	O	ASN	B	383	56.024	127.038	149.524	1.00	98.35
	1980	N	HIS	B	384	56.937	126.189	147.668	1.00	93.62
	1981	CA	HIS	B	384	55.806	125.312	147.411	1.00	67.76
5	1982	CB	HIS	B	384	55.861	124.821	145.971	1.00	86.21
	1983	CG	HIS	B	384	55.759	125.923	144.968	1.00	106.64
	1984	CD2	HIS	B	384	56.710	126.691	144.388	1.00	118.02
	1985	ND1	HIS	B	384	54.551	126.390	144.500	1.00	70.58
	1986	CE1	HIS	B	384	54.760	127.398	143.676	1.00	107.89
10	1987	NE2	HIS	B	384	56.063	127.602	143.590	1.00	141.17
	1988	C	HIS	B	384	55.859	124.145	148.392	1.00	78.76
	1989	O	HIS	B	384	56.936	123.688	148.786	1.00	62.48
	1990	N	SER	B	385	54.694	123.665	148.801	1.00	90.92
	1991	CA	SER	B	385	54.650	122.571	149.760	1.00	50.91
15	1992	CB	SER	B	385	53.664	122.908	150.880	1.00	71.25
	1993	OG	SER	B	385	52.375	123.192	150.354	1.00	104.23
	1994	C	SER	B	385	54.271	121.242	149.136	1.00	72.39
	1995	O	SER	B	385	53.913	121.162	147.955	1.00	65.67
	1996	N	THR	B	386	54.359	120.210	149.970	1.00	62.20
20	1997	CA	THR	B	386	54.036	118.826	149.632	1.00	53.65
	1998	CB	THR	B	386	55.117	117.911	150.210	1.00	90.34
	1999	OG1	THR	B	386	56.193	117.804	149.269	1.00	80.69
	2000	CG2	THR	B	386	54.552	116.533	150.571	1.00	100.14
	2001	C	THR	B	386	52.684	118.468	150.266	1.00	68.47
25	2002	O	THR	B	386	52.200	119.188	151.139	1.00	105.23
	2003	N	ARG	B	387	52.063	117.377	149.837	1.00	56.81
	2004	CA	ARG	B	387	50.795	117.008	150.437	1.00	54.80
	2005	CB	ARG	B	387	49.720	118.013	150.006	1.00	49.15
	2006	CG	ARG	B	387	48.321	117.671	150.466	1.00	66.87
30	2007	CD	ARG	B	387	47.403	118.853	150.339	1.00	67.37
	2008	NE	ARG	B	387	46.030	118.490	150.645	1.00	77.86
	2009	CZ	ARG	B	387	45.055	119.376	150.780	1.00	111.21
	2010	NH1	ARG	B	387	45.318	120.669	150.633	1.00	100.94
	2011	NH2	ARG	B	387	43.825	118.971	151.064	1.00	96.41
35	2012	C	ARG	B	387	50.347	115.582	150.128	1.00	56.65
	2013	O	ARG	B	387	50.294	115.184	148.963	1.00	61.16
	2014	N	LYS	B	388	50.035	114.816	151.177	1.00	36.92
	2015	CA	LYS	B	388	49.555	113.441	151.016	1.00	59.67
	2016	CB	LYS	B	388	50.560	112.426	151.556	1.00	30.37
40	2017	CG	LYS	B	388	52.019	112.796	151.452	1.00	148.33
	2018	CD	LYS	B	388	52.864	111.704	152.106	1.00	145.55
	2019	CE	LYS	B	388	54.353	112.005	152.019	1.00	171.95
	2020	NZ	LYS	B	388	55.174	110.852	152.491	1.00	153.54
	2021	C	LYS	B	388	48.290	113.253	151.835	1.00	56.48
45	2022	O	LYS	B	388	48.189	113.793	152.938	1.00	73.87
	2023	N	GLU	B	389	47.339	112.480	151.324	1.00	33.78
	2024	CA	GLU	B	389	46.120	112.216	152.086	1.00	52.94
	2025	CB	GLU	B	389	44.889	112.865	151.423	1.00	32.75
	2026	CG	GLU	B	389	44.856	114.388	151.542	1.00	138.12
50	2027	CD	GLU	B	389	43.709	115.017	150.776	1.00	167.38
	2028	OE1	GLU	B	389	42.548	114.596	150.983	1.00	151.81
	2029	OE2	GLU	B	389	43.977	115.938	149.971	1.00	152.33
	2030	C	GLU	B	389	45.927	110.715	152.197	1.00	54.81
	2031	O	GLU	B	389	45.401	110.088	151.280	1.00	91.54
55	2032	N	GLU	B	390	46.345	110.143	153.321	1.00	39.47

	2033	CA	GLU	B	390	46.227	108.705	153.522	1.00	78.09
	2034	CB	GLU	B	390	47.466	108.168	154.252	1.00	97.18
	2035	CG	GLU	B	390	48.812	108.585	153.679	1.00	148.70
	2036	CD	GLU	B	390	49.982	107.940	154.417	1.00	168.33
	2037	OE1	GLU	B	390	50.020	108.020	155.666	1.00	162.95
	2038	OE2	GLU	B	390	50.866	107.358	153.747	1.00	166.90
	2039	C	GLU	B	390	45.000	108.231	154.301	1.00	24.57
	2040	O	GLU	B	390	44.928	108.435	155.504	1.00	58.87
	2041	N	LYS	B	391	44.046	107.581	153.638	1.00	39.47
	2042	CA	LYS	B	391	42.892	107.033	154.357	1.00	36.12
	2043	CB	LYS	B	391	41.939	106.319	153.392	1.00	30.68
	2044	CG	LYS	B	391	40.901	105.431	154.103	1.00	91.41
	2045	CD	LYS	B	391	40.563	104.141	153.322	1.00	153.55
	2046	CE	LYS	B	391	39.785	104.403	152.029	1.00	171.40
	2047	NZ	LYS	B	391	39.360	103.133	151.353	1.00	125.88
	2048	C	LYS	B	391	43.471	106.004	155.342	1.00	35.98
	2049	O	LYS	B	391	44.138	105.064	154.925	1.00	52.90
	2050	N	GLN	B	392	43.232	106.173	156.636	1.00	47.33
	2051	CA	GLN	B	392	43.778	105.248	157.617	1.00	50.54
	2052	CB	GLN	B	392	44.026	105.955	158.932	1.00	52.52
	2053	CG	GLN	B	392	44.910	107.158	158.819	1.00	43.19
	2054	CD	GLN	B	392	46.307	106.799	158.433	1.00	52.17
	2055	OE1	GLN	B	392	46.549	106.342	157.315	1.00	140.45
	2056	NE2	GLN	B	392	47.251	106.987	159.354	1.00	104.37
	2057	C	GLN	B	392	42.876	104.062	157.857	1.00	83.18
	2058	O	GLN	B	392	41.730	104.057	157.421	1.00	48.10
	2059	N	ARG	B	393	43.396	103.069	158.573	1.00	86.36
	2060	CA	ARG	B	393	42.646	101.853	158.851	1.00	95.47
	2061	CB	ARG	B	393	43.537	100.804	159.528	1.00	129.48
	2062	CG	ARG	B	393	42.798	99.515	159.903	1.00	156.47
	2063	CD	ARG	B	393	43.235	98.309	159.074	1.00	159.01
	2064	NE	ARG	B	393	44.594	97.884	159.395	1.00	164.37
	2065	CZ	ARG	B	393	45.164	96.782	158.918	1.00	170.49
	2066	NH1	ARG	B	393	44.492	95.988	158.094	1.00	168.61
	2067	NH2	ARG	B	393	46.408	96.474	159.267	1.00	175.65
	2068	C	ARG	B	393	41.421	102.083	159.704	1.00	67.02
	2069	O	ARG	B	393	40.379	101.483	159.461	1.00	85.39
	2070	N	ASN	B	394	41.532	102.952	160.702	1.00	92.32
	2071	CA	ASN	B	394	40.400	103.198	161.591	1.00	86.89
	2072	CB	ASN	B	394	40.867	103.749	162.953	1.00	80.23
	2073	CG	ASN	B	394	41.534	105.117	162.866	1.00	40.68
	2074	OD1	ASN	B	394	41.174	105.955	162.053	1.00	63.47
	2075	ND2	ASN	B	394	42.490	105.336	163.761	1.00	63.72
	2076	C	ASN	B	394	39.286	104.073	161.044	1.00	37.93
	2077	O	ASN	B	394	38.610	104.750	161.788	1.00	46.38
	2078	N	GLY	B	395	39.075	104.048	159.740	1.00	70.31
	2079	CA	GLY	B	395	38.004	104.853	159.177	1.00	65.82
	2080	C	GLY	B	395	38.289	106.338	159.044	1.00	31.15
	2081	O	GLY	B	395	37.619	107.040	158.285	1.00	51.28
	2082	N	THR	B	396	39.286	106.822	159.774	1.00	53.28
	2083	CA	THR	B	396	39.642	108.226	159.712	1.00	40.78
	2084	CB	THR	B	396	40.600	108.599	160.829	1.00	19.53
	2085	OG1	THR	B	396	40.696	110.023	160.904	1.00	154.97
	2086	CG2	THR	B	396	41.976	108.064	160.557	1.00	109.19
	2087	C	THR	B	396	40.296	108.573	158.383	1.00	40.28

	2088	O	THR	B	396	40.205	107.818	157.422	1.00	73.66
	2089	N	LEU	B	397	40.965	109.719	158.342	1.00	34.73
	2090	CA	LEU	B	397	41.643	110.210	157.146	1.00	43.25
	2091	CB	LEU	B	397	40.643	110.871	156.211	1.00	57.03
	2092	CG	LEU	B	397	41.194	111.797	155.133	1.00	45.14
	2093	CD1	LEU	B	397	42.136	111.032	154.228	1.00	110.61
	2094	CD2	LEU	B	397	40.032	112.353	154.322	1.00	106.87
	2095	C	LEU	B	397	42.678	111.231	157.579	1.00	52.48
	2096	O	LEU	B	397	42.351	112.181	158.271	1.00	67.73
	2097	N	THR	B	398	43.925	111.027	157.166	1.00	62.48
	2098	CA	THR	B	398	45.033	111.910	157.522	1.00	36.96
	2099	CB	THR	B	398	46.226	111.106	158.025	1.00	17.60
	2100	OG1	THR	B	398	45.893	110.477	159.258	1.00	49.11
	2101	CG2	THR	B	398	47.409	111.998	158.248	1.00	64.17
	2102	C	THR	B	398	45.524	112.775	156.373	1.00	32.07
	2103	O	THR	B	398	45.349	112.449	155.208	1.00	60.40
	2104	N	VAL	B	399	46.156	113.882	156.725	1.00	24.42
	2105	CA	VAL	B	399	46.695	114.800	155.749	1.00	35.05
	2106	CB	VAL	B	399	45.788	116.004	155.569	1.00	18.51
	2107	CG1	VAL	B	399	46.501	117.089	154.798	1.00	27.22
	2108	CG2	VAL	B	399	44.534	115.572	154.853	1.00	29.70
	2109	C	VAL	B	399	48.011	115.300	156.268	1.00	43.68
	2110	O	VAL	B	399	48.063	115.809	157.380	1.00	42.74
	2111	N	THR	B	400	49.082	115.139	155.495	1.00	53.46
	2112	CA	THR	B	400	50.377	115.663	155.927	1.00	43.16
	2113	CB	THR	B	400	51.450	114.598	156.085	1.00	42.86
	2114	OG1	THR	B	400	51.697	114.011	154.813	1.00	69.60
	2115	CG2	THR	B	400	51.014	113.532	157.036	1.00	42.99
	2116	C	THR	B	400	50.862	116.598	154.844	1.00	51.26
	2117	O	THR	B	400	50.595	116.382	153.656	1.00	66.11
	2118	N	SER	B	401	51.573	117.637	155.261	1.00	47.73
	2119	CA	SER	B	401	52.117	118.610	154.333	1.00	44.60
	2120	CB	SER	B	401	51.199	119.817	154.209	1.00	50.71
	2121	OG	SER	B	401	51.810	120.856	153.475	1.00	40.79
	2122	C	SER	B	401	53.457	119.052	154.862	1.00	58.39
	2123	O	SER	B	401	53.551	119.546	155.993	1.00	37.36
	2124	N	THR	B	402	54.495	118.859	154.048	1.00	77.89
	2125	CA	THR	B	402	55.840	119.241	154.442	1.00	61.20
	2126	CB	THR	B	402	56.821	118.125	154.152	1.00	61.85
	2127	OG1	THR	B	402	56.295	116.895	154.661	1.00	81.37
	2128	CG2	THR	B	402	58.157	118.409	154.814	1.00	109.89
	2129	C	THR	B	402	56.242	120.481	153.672	1.00	68.43
	2130	O	THR	B	402	55.879	120.648	152.496	1.00	56.79
	2131	N	LEU	B	403	56.991	121.354	154.339	1.00	62.35
	2132	CA	LEU	B	403	57.413	122.599	153.719	1.00	65.76
	2133	CB	LEU	B	403	56.613	123.752	154.320	1.00	66.45
	2134	CG	LEU	B	403	56.909	125.152	153.790	1.00	75.07
	2135	CD1	LEU	B	403	56.506	125.263	152.324	1.00	107.93
	2136	CD2	LEU	B	403	56.167	126.156	154.629	1.00	75.06
	2137	C	LEU	B	403	58.912	122.897	153.838	1.00	92.32
	2138	O	LEU	B	403	59.488	122.821	154.932	1.00	34.92
	2139	N	PRO	B	404	59.556	123.238	152.702	1.00	49.08
	2140	CD	PRO	B	404	58.975	123.180	151.351	1.00	61.61
	2141	CA	PRO	B	404	60.976	123.560	152.621	1.00	52.97
	2142	CB	PRO	B	404	61.220	123.656	151.121	1.00	111.63

	2143	CG	PRO	B	404	60.157	122.787	150.539	1.00	84.92
	2144	C	PRO	B	404	61.217	124.891	153.310	1.00	73.53
	2145	O	PRO	B	404	60.473	125.843	153.112	1.00	63.87
	2146	N	VAL	B	405	62.282	124.975	154.087	1.00	86.35
	2147	CA	VAL	B	405	62.543	126.198	154.812	1.00	76.26
	2148	CB	VAL	B	405	62.100	126.000	156.269	1.00	36.70
	2149	CG1	VAL	B	405	63.203	126.416	157.230	1.00	127.12
	2150	CG2	VAL	B	405	60.845	126.775	156.513	1.00	88.70
	2151	C	VAL	B	405	63.982	126.712	154.754	1.00	107.63
	2152	O	VAL	B	405	64.940	125.951	154.939	1.00	91.98
	2153	N	GLY	B	406	64.113	128.017	154.509	1.00	73.83
	2154	CA	GLY	B	406	65.427	128.645	154.435	1.00	131.05
	2155	C	GLY	B	406	66.225	128.509	155.736	1.00	130.39
	2156	O	GLY	B	406	65.896	129.124	156.744	1.00	100.56
	2157	N	THR	B	407	67.292	127.716	155.688	1.00	142.82
	2158	CA	THR	B	407	68.143	127.461	156.830	1.00	100.01
	2159	CB	THR	B	407	69.482	126.859	156.428	1.00	126.91
	2160	OG1	THR	B	407	69.350	126.170	155.184	1.00	151.73
	2161	CG2	THR	B	407	69.964	125.900	157.521	1.00	85.87
	2162	C	THR	B	407	68.488	128.714	157.631	1.00	111.52
	2163	O	THR	B	407	68.563	128.679	158.858	1.00	92.93
	2164	N	ARG	B	408	68.734	129.816	156.934	1.00	135.67
	2165	CA	ARG	B	408	69.098	131.063	157.590	1.00	137.76
	2166	CB	ARG	B	408	69.517	132.097	156.546	1.00	153.22
	2167	CG	ARG	B	408	70.749	131.688	155.715	1.00	174.72
	2168	CD	ARG	B	408	70.530	130.402	154.906	1.00	170.05
	2169	NE	ARG	B	408	69.575	130.568	153.813	1.00	157.68
	2170	CZ	ARG	B	408	69.164	129.575	153.031	1.00	144.79
	2171	NH1	ARG	B	408	69.617	128.342	153.226	1.00	99.09
	2172	NH2	ARG	B	408	68.314	129.818	152.043	1.00	134.60
	2173	C	ARG	B	408	67.905	131.589	158.374	1.00	125.74
	2174	O	ARG	B	408	67.885	131.590	159.622	1.00	107.88
	2175	N	ASP	B	409	66.897	132.018	157.626	1.00	114.38
	2176	CA	ASP	B	409	65.665	132.577	158.171	1.00	100.02
	2177	CB	ASP	B	409	64.547	132.393	157.129	1.00	106.65
	2178	CG	ASP	B	409	64.925	132.915	155.743	1.00	131.77
	2179	OD1	ASP	B	409	64.961	134.151	155.545	1.00	128.42
	2180	OD2	ASP	B	409	65.187	132.086	154.841	1.00	107.93
	2181	C	ASP	B	409	65.242	131.954	159.503	1.00	87.73
	2182	O	ASP	B	409	64.932	132.667	160.459	1.00	125.50
	2183	N	TRP	B	410	65.229	130.626	159.553	1.00	82.03
	2184	CA	TRP	B	410	64.836	129.888	160.749	1.00	68.60
	2185	CB	TRP	B	410	64.923	128.385	160.486	1.00	79.72
	2186	CG	TRP	B	410	64.743	127.540	161.706	1.00	47.85
	2187	CD2	TRP	B	410	63.509	127.028	162.201	1.00	87.88
	2188	CE2	TRP	B	410	63.796	126.300	163.380	1.00	73.32
	2189	CE3	TRP	B	410	62.184	127.117	161.764	1.00	50.59
	2190	CD1	TRP	B	410	65.711	127.116	162.577	1.00	100.57
	2191	NE1	TRP	B	410	65.147	126.367	163.587	1.00	53.96
	2192	CZ2	TRP	B	410	62.806	125.668	164.127	1.00	90.94
	2193	CZ3	TRP	B	410	61.203	126.490	162.505	1.00	42.94
	2194	CH2	TRP	B	410	61.517	125.773	163.678	1.00	64.03
	2195	C	TRP	B	410	65.675	130.226	161.960	1.00	98.97
	2196	O	TRP	B	410	65.141	130.650	162.976	1.00	129.24
	2197	N	ILE	B	411	66.985	130.031	161.860	1.00	106.60

	2198	CA	ILE	B	411	67.850	130.306	162.998	1.00	115.95
	2199	CB	ILE	B	411	69.317	130.062	162.670	1.00	103.18
	2200	CG2	ILE	B	411	70.075	129.721	163.955	1.00	112.78
	2201	CG1	ILE	B	411	69.438	128.905	161.683	1.00	127.25
5	2202	CD1	ILE	B	411	70.843	128.694	161.174	1.00	162.43
	2203	C	ILE	B	411	67.701	131.744	163.459	1.00	130.64
	2204	O	ILE	B	411	67.892	132.055	164.637	1.00	115.79
	2205	N	GLU	B	412	67.359	132.627	162.529	1.00	89.59
	2206	CA	GLU	B	412	67.183	134.023	162.883	1.00	115.46
10	2207	CB	GLU	B	412	67.480	134.912	161.677	1.00	137.38
	2208	CG	GLU	B	412	68.974	135.047	161.407	1.00	156.60
	2209	CD	GLU	B	412	69.283	136.016	160.288	1.00	185.08
	2210	OE1	GLU	B	412	68.761	137.150	160.329	1.00	188.44
	2211	OE2	GLU	B	412	70.051	135.648	159.374	1.00	188.13
15	2212	C	GLU	B	412	65.799	134.316	163.458	1.00	140.17
	2213	O	GLU	B	412	65.262	135.411	163.299	1.00	136.77
	2214	N	GLY	B	413	65.228	133.314	164.121	1.00	164.88
	2215	CA	GLY	B	413	63.931	133.461	164.761	1.00	159.55
	2216	C	GLY	B	413	62.653	133.570	163.947	1.00	139.70
20	2217	O	GLY	B	413	61.592	133.808	164.523	1.00	138.95
	2218	N	GLU	B	414	62.720	133.404	162.631	1.00	131.17
	2219	CA	GLU	B	414	61.509	133.499	161.824	1.00	96.50
	2220	CB	GLU	B	414	61.778	133.066	160.389	1.00	107.97
	2221	CG	GLU	B	414	60.530	132.974	159.525	1.00	80.41
25	2222	CD	GLU	B	414	59.820	134.291	159.380	1.00	87.05
	2223	OE1	GLU	B	414	59.242	134.775	160.373	1.00	111.31
	2224	OE2	GLU	B	414	59.847	134.849	158.265	1.00	93.50
	2225	C	GLU	B	414	60.420	132.622	162.423	1.00	101.40
	2226	O	GLU	B	414	60.687	131.784	163.285	1.00	104.23
30	2227	N	THR	B	415	59.192	132.819	161.960	1.00	115.03
	2228	CA	THR	B	415	58.056	132.059	162.458	1.00	112.22
	2229	CB	THR	B	415	57.348	132.843	163.575	1.00	118.03
	2230	OG1	THR	B	415	55.994	132.403	163.687	1.00	110.64
	2231	CG2	THR	B	415	57.422	134.334	163.313	1.00	155.73
35	2232	C	THR	B	415	57.055	131.660	161.366	1.00	127.06
	2233	O	THR	B	415	56.517	132.506	160.626	1.00	84.52
	2234	N	TYR	B	416	56.818	130.351	161.282	1.00	115.33
	2235	CA	TYR	B	416	55.922	129.765	160.287	1.00	76.98
	2236	CB	TYR	B	416	56.626	128.606	159.569	1.00	86.80
40	2237	CG	TYR	B	416	57.961	128.956	158.940	1.00	94.67
	2238	CD1	TYR	B	416	59.155	128.835	159.662	1.00	110.20
	2239	CE1	TYR	B	416	60.380	129.198	159.099	1.00	47.43
	2240	CD2	TYR	B	416	58.024	129.446	157.635	1.00	61.95
	2241	CE2	TYR	B	416	59.231	129.815	157.066	1.00	64.97
45	2242	CZ	TYR	B	416	60.408	129.693	157.797	1.00	90.31
	2243	OH	TYR	B	416	61.601	130.081	157.222	1.00	162.34
	2244	C	TYR	B	416	54.623	129.255	160.897	1.00	92.23
	2245	O	TYR	B	416	54.604	128.778	162.041	1.00	59.60
	2246	N	GLN	B	417	53.546	129.322	160.115	1.00	62.55
50	2247	CA	GLN	B	417	52.236	128.889	160.592	1.00	50.69
	2248	CB	GLN	B	417	51.411	130.114	160.969	1.00	129.83
	2249	CG	GLN	B	417	50.127	129.811	161.708	1.00	147.33
	2250	CD	GLN	B	417	49.282	131.051	161.924	1.00	140.76
	2251	OE1	GLN	B	417	48.740	131.624	160.971	1.00	120.92
55	2252	NE2	GLN	B	417	49.167	131.477	163.181	1.00	129.75

	2253	C	GLN	B	417	51.457	128.058	159.575	1.00	59.75
	2254	O	GLN	B	417	51.437	128.363	158.381	1.00	76.03
	2255	N	CYS	B	418	50.796	127.018	160.080	1.00	69.24
	2256	CA	CYS	B	418	49.998	126.095	159.267	1.00	63.48
	2257	C	CYS	B	418	48.521	126.354	159.532	1.00	71.26
	2258	O	CYS	B	418	48.083	126.288	160.688	1.00	66.93
	2259	CB	CYS	B	418	50.343	124.647	159.636	1.00	83.48
	2260	SG	CYS	B	418	49.465	123.360	158.682	1.00	121.42
	2261	N	ARG	B	419	47.756	126.640	158.474	1.00	40.08
	2262	CA	ARG	B	419	46.327	126.928	158.637	1.00	38.15
	2263	CB	ARG	B	419	46.008	128.369	158.211	1.00	106.47
	2264	CG	ARG	B	419	44.562	128.797	158.483	1.00	184.87
	2265	CD	ARG	B	419	44.235	130.164	157.902	1.00	224.39
	2266	NE	ARG	B	419	42.880	130.587	158.248	1.00	235.46
	2267	CZ	ARG	B	419	42.299	131.685	157.782	1.00	221.27
	2268	NH1	ARG	B	419	42.952	132.475	156.945	1.00	212.86
	2269	NH2	ARG	B	419	41.067	131.995	158.156	1.00	204.55
	2270	C	ARG	B	419	45.434	125.975	157.868	1.00	66.29
	2271	O	ARG	B	419	45.318	126.081	156.658	1.00	49.15
	2272	N	VAL	B	420	44.777	125.056	158.565	1.00	41.47
	2273	CA	VAL	B	420	43.891	124.107	157.877	1.00	57.57
	2274	CB	VAL	B	420	44.050	122.684	158.466	1.00	53.54
	2275	CG1	VAL	B	420	45.434	122.539	159.084	1.00	58.35
	2276	CG2	VAL	B	420	42.980	122.416	159.517	1.00	71.65
	2277	C	VAL	B	420	42.439	124.602	158.000	1.00	50.86
	2278	O	VAL	B	420	42.085	125.213	159.020	1.00	51.31
	2279	N	THR	B	421	41.636	124.307	156.966	1.00	31.63
	2280	CA	THR	B	421	40.259	124.752	156.844	1.00	41.77
	2281	CB	THR	B	421	40.214	126.119	156.170	1.00	12.47
	2282	OG1	THR	B	421	40.364	127.127	157.168	1.00	107.15
	2283	CG2	THR	B	421	38.907	126.314	155.393	1.00	70.23
	2284	C	THR	B	421	39.294	123.902	156.029	1.00	49.50
	2285	O	THR	B	421	39.438	123.788	154.818	1.00	60.59
	2286	N	HIS	B	422	38.259	123.357	156.640	1.00	61.87
	2287	CA	HIS	B	422	37.333	122.547	155.856	1.00	46.82
	2288	CB	HIS	B	422	37.688	121.069	156.046	1.00	54.88
	2289	CG	HIS	B	422	36.899	120.137	155.186	1.00	66.28
	2290	CD2	HIS	B	422	36.786	120.023	153.852	1.00	90.39
	2291	ND1	HIS	B	422	36.142	119.123	155.730	1.00	105.82
	2292	CE1	HIS	B	422	35.595	118.426	154.754	1.00	67.94
	2293	NE2	HIS	B	422	35.968	118.950	153.598	1.00	89.25
	2294	C	HIS	B	422	35.883	122.789	156.278	1.00	35.50
	2295	O	HIS	B	422	35.615	123.100	157.427	1.00	63.71
	2296	N	PRO	B	423	34.938	122.661	155.333	1.00	33.86
	2297	CD	PRO	B	423	35.231	122.574	153.889	1.00	61.95
	2298	CA	PRO	B	423	33.500	122.844	155.563	1.00	74.49
	2299	CB	PRO	B	423	32.892	122.227	154.320	1.00	30.75
	2300	CG	PRO	B	423	33.833	122.723	153.266	1.00	92.20
	2301	C	PRO	B	423	33.024	122.170	156.843	1.00	25.99
	2302	O	PRO	B	423	32.254	122.745	157.604	1.00	94.74
	2303	N	HIS	B	424	33.489	120.951	157.078	1.00	72.49
	2304	CA	HIS	B	424	33.139	120.178	158.262	1.00	35.64
	2305	CB	HIS	B	424	33.886	118.850	158.263	1.00	68.85
	2306	CG	HIS	B	424	33.378	117.865	157.264	1.00	33.77
	2307	CD2	HIS	B	424	32.613	118.022	156.163	1.00	93.93

	2308	ND1	HIS	B	424	33.632	116.516	157.368	1.00	22.18
	2309	CE1	HIS	B	424	33.043	115.883	156.373	1.00	72.12
	2310	NE2	HIS	B	424	32.417	116.774	155.626	1.00	92.83
	2311	C	HIS	B	424	33.562	120.919	159.503	1.00	72.43
5	2312	O	HIS	B	424	33.155	120.583	160.614	1.00	45.64
	2313	N	LEU	B	425	34.397	121.925	159.310	1.00	30.28
	2314	CA	LEU	B	425	34.907	122.679	160.429	1.00	67.62
	2315	CB	LEU	B	425	36.415	122.774	160.284	1.00	51.81
	2316	CG	LEU	B	425	37.061	121.393	160.189	1.00	50.51
10	2317	CD1	LEU	B	425	38.563	121.538	160.155	1.00	99.40
	2318	CD2	LEU	B	425	36.651	120.562	161.377	1.00	41.28
	2319	C	LEU	B	425	34.323	124.059	160.708	1.00	63.27
	2320	O	LEU	B	425	34.105	124.859	159.800	1.00	102.78
	2321	N	PRO	B	426	34.071	124.348	161.994	1.00	57.60
15	2322	CD	PRO	B	426	34.288	123.365	163.068	1.00	65.15
	2323	CA	PRO	B	426	33.523	125.589	162.550	1.00	52.46
	2324	CB	PRO	B	426	33.167	125.178	163.965	1.00	85.27
	2325	CG	PRO	B	426	34.270	124.230	164.292	1.00	34.92
	2326	C	PRO	B	426	34.576	126.710	162.531	1.00	49.56
20	2327	O	PRO	B	426	34.524	127.605	161.692	1.00	85.61
	2328	N	ARG	B	427	35.513	126.657	163.475	1.00	56.31
	2329	CA	ARG	B	427	36.606	127.626	163.550	1.00	81.37
	2330	CB	ARG	B	427	37.101	127.788	165.016	1.00	37.35
	2331	CG	ARG	B	427	37.494	126.478	165.701	1.00	67.67
25	2332	CD	ARG	B	427	37.021	126.334	167.163	1.00	106.61
	2333	NE	ARG	B	427	36.476	124.989	167.420	1.00	156.12
	2334	CZ	ARG	B	427	36.257	124.464	168.627	1.00	157.58
	2335	NH1	ARG	B	427	36.543	125.167	169.717	1.00	155.60
	2336	NH2	ARG	B	427	35.737	123.236	168.748	1.00	66.93
30	2337	C	ARG	B	427	37.709	127.037	162.664	1.00	71.40
	2338	O	ARG	B	427	37.641	125.876	162.279	1.00	38.48
	2339	N	ALA	B	428	38.713	127.824	162.313	1.00	105.95
	2340	CA	ALA	B	428	39.793	127.289	161.495	1.00	47.56
	2341	CB	ALA	B	428	40.458	128.403	160.734	1.00	123.77
35	2342	C	ALA	B	428	40.782	126.651	162.451	1.00	60.43
	2343	O	ALA	B	428	40.721	126.891	163.651	1.00	68.94
	2344	N	LEU	B	429	41.689	125.836	161.932	1.00	64.23
	2345	CA	LEU	B	429	42.698	125.194	162.769	1.00	63.17
	2346	CB	LEU	B	429	42.750	123.697	162.523	1.00	33.26
40	2347	CG	LEU	B	429	42.661	122.872	163.803	1.00	88.80
	2348	CD1	LEU	B	429	42.937	121.426	163.444	1.00	60.45
	2349	CD2	LEU	B	429	43.645	123.380	164.857	1.00	119.69
	2350	C	LEU	B	429	44.041	125.779	162.418	1.00	60.60
	2351	O	LEU	B	429	44.392	125.847	161.247	1.00	46.41
45	2352	N	MET	B	430	44.792	126.186	163.433	1.00	45.54
	2353	CA	MET	B	430	46.085	126.789	163.209	1.00	42.39
	2354	CB	MET	B	430	46.004	128.321	163.336	1.00	51.46
	2355	CG	MET	B	430	45.156	129.011	162.277	1.00	72.95
	2356	SD	MET	B	430	45.247	130.811	162.351	1.00	135.30
50	2357	CE	MET	B	430	44.061	131.159	163.665	1.00	161.36
	2358	C	MET	B	430	47.063	126.286	164.226	1.00	61.09
	2359	O	MET	B	430	46.686	125.890	165.335	1.00	52.58
	2360	N	ARG	B	431	48.326	126.285	163.821	1.00	42.23
	2361	CA	ARG	B	431	49.423	125.906	164.696	1.00	63.07
55	2362	CB	ARG	B	431	49.602	124.404	164.736	1.00	33.42

	2363	CG	ARG	B	431	48.302	123.660	164.986	1.00	57.91
	2364	CD	ARG	B	431	48.510	122.413	165.816	1.00	51.62
	2365	NE	ARG	B	431	48.125	122.644	167.201	1.00	93.78
	2366	CZ	ARG	B	431	46.876	122.871	167.585	1.00	101.45
5	2367	NH1	ARG	B	431	45.907	122.888	166.681	1.00	36.13
	2368	NH2	ARG	B	431	46.601	123.088	168.865	1.00	161.49
	2369	C	ARG	B	431	50.627	126.588	164.085	1.00	72.59
	2370	O	ARG	B	431	50.663	126.820	162.869	1.00	53.93
	2371	N	SER	B	432	51.589	126.941	164.928	1.00	70.72
10	2372	CA	SER	B	432	52.772	127.634	164.457	1.00	71.54
	2373	CB	SER	B	432	52.625	129.138	164.671	1.00	72.40
	2374	OG	SER	B	432	52.566	129.443	166.058	1.00	106.30
	2375	C	SER	B	432	53.974	127.142	165.224	1.00	99.13
	2376	O	SER	B	432	53.831	126.433	166.226	1.00	55.86
15	2377	N	THR	B	433	55.155	127.529	164.749	1.00	84.30
	2378	CA	THR	B	433	56.400	127.130	165.384	1.00	88.35
	2379	CB	THR	B	433	56.722	125.683	165.096	1.00	76.49
	2380	OG1	THR	B	433	57.898	125.303	165.820	1.00	105.68
	2381	CG2	THR	B	433	56.953	125.506	163.607	1.00	49.60
20	2382	C	THR	B	433	57.567	127.947	164.891	1.00	97.22
	2383	O	THR	B	433	57.576	128.410	163.734	1.00	66.32
	2384	N	THR	B	434	58.546	128.111	165.785	1.00	77.69
	2385	CA	THR	B	434	59.786	128.838	165.511	1.00	65.57
	2386	CB	THR	B	434	59.687	130.335	165.820	1.00	84.37
25	2387	OG1	THR	B	434	59.875	130.555	167.229	1.00	140.54
	2388	CG2	THR	B	434	58.342	130.886	165.421	1.00	65.31
	2389	C	THR	B	434	60.880	128.307	166.436	1.00	96.20
	2390	O	THR	B	434	60.621	127.548	167.360	1.00	67.43
	2391	N	LYS	B	435	62.095	128.750	166.146	1.00	102.83
30	2392	CA	LYS	B	435	63.296	128.401	166.859	1.00	94.54
	2393	CB	LYS	B	435	64.392	129.385	166.468	1.00	102.66
	2394	CG	LYS	B	435	65.736	129.328	167.181	1.00	156.34
	2395	CD	LYS	B	435	66.662	130.374	166.492	1.00	155.89
	2396	CE	LYS	B	435	68.100	130.543	167.040	1.00	174.55
35	2397	NZ	LYS	B	435	68.097	131.005	168.483	1.00	180.88
	2398	C	LYS	B	435	63.073	128.443	168.369	1.00	90.68
	2399	O	LYS	B	435	62.554	129.421	168.898	1.00	125.40
	2400	N	THR	B	436	63.449	127.383	169.070	1.00	65.76
	2401	CA	THR	B	436	63.293	127.351	170.526	1.00	80.29
40	2402	CB	THR	B	436	63.710	126.002	171.078	1.00	74.52
	2403	OG1	THR	B	436	63.054	124.968	170.344	1.00	133.68
	2404	CG2	THR	B	436	63.341	125.879	172.532	1.00	84.46
	2405	C	THR	B	436	64.159	128.429	171.186	1.00	132.09
	2406	O	THR	B	436	65.294	128.670	170.764	1.00	135.39
45	2407	N	SER	B	437	63.639	129.031	172.255	1.00	135.64
	2408	CA	SER	B	437	64.341	130.112	172.957	1.00	154.94
	2409	CB	SER	B	437	63.334	131.187	173.370	1.00	159.96
	2410	OG	SER	B	437	62.326	130.634	174.204	1.00	151.19
	2411	C	SER	B	437	65.157	129.701	174.176	1.00	145.96
50	2412	O	SER	B	437	65.253	128.518	174.505	1.00	126.88
	2413	N	GLY	B	438	65.748	130.698	174.834	1.00	142.79
	2414	CA	GLY	B	438	66.544	130.446	176.022	1.00	127.41
	2415	C	GLY	B	438	68.046	130.551	175.823	1.00	105.05
	2416	O	GLY	B	438	68.511	131.074	174.814	1.00	92.39
55	2417	N	PRO	B	439	68.836	130.081	176.796	1.00	96.54

	2418	CD	PRO	B	439	68.372	129.693	178.137	1.00	102.85
	2419	CA	PRO	B	439	70.299	130.103	176.748	1.00	119.07
	2420	CB	PRO	B	439	70.684	130.075	178.218	1.00	146.55
	2421	CG	PRO	B	439	69.637	129.177	178.787	1.00	118.33
5	2422	C	PRO	B	439	70.807	128.876	175.989	1.00	126.07
	2423	O	PRO	B	439	70.310	127.768	176.199	1.00	134.45
	2424	N	ARG	B	440	71.805	129.094	175.127	1.00	120.46
	2425	CA	ARG	B	440	72.374	128.039	174.291	1.00	111.19
	2426	CB	ARG	B	440	72.576	128.565	172.866	1.00	122.47
10	2427	CG	ARG	B	440	71.504	129.538	172.390	1.00	147.23
	2428	CD	ARG	B	440	70.181	128.851	172.101	1.00	186.68
	2429	NE	ARG	B	440	69.065	129.796	172.154	1.00	214.53
	2430	CZ	ARG	B	440	67.972	129.726	171.400	1.00	221.94
	2431	NH1	ARG	B	440	67.829	128.750	170.511	1.00	219.20
15	2432	NH2	ARG	B	440	67.023	130.642	171.541	1.00	205.02
	2433	C	ARG	B	440	73.699	127.481	174.812	1.00	89.64
	2434	O	ARG	B	440	74.753	128.090	174.628	1.00	132.22
	2435	N	ALA	B	441	73.650	126.315	175.450	1.00	73.11
	2436	CA	ALA	B	441	74.869	125.692	175.965	1.00	83.71
20	2437	CB	ALA	B	441	74.701	125.340	177.430	1.00	94.78
	2438	C	ALA	B	441	75.217	124.441	175.151	1.00	85.35
	2439	O	ALA	B	441	74.409	123.514	175.047	1.00	93.65
	2440	N	ALA	B	442	76.430	124.427	174.595	1.00	115.97
	2441	CA	ALA	B	442	76.938	123.321	173.775	1.00	86.76
25	2442	CB	ALA	B	442	78.341	123.654	173.274	1.00	132.70
	2443	C	ALA	B	442	76.946	121.954	174.466	1.00	93.35
	2444	O	ALA	B	442	76.879	121.858	175.693	1.00	88.94
	2445	N	PRO	B	443	77.045	120.877	173.670	1.00	88.73
	2446	CD	PRO	B	443	76.967	120.894	172.202	1.00	53.59
30	2447	CA	PRO	B	443	77.057	119.497	174.160	1.00	66.28
	2448	CB	PRO	B	443	76.504	118.696	172.982	1.00	75.52
	2449	CG	PRO	B	443	76.059	119.745	171.951	1.00	82.83
	2450	C	PRO	B	443	78.413	118.970	174.561	1.00	69.00
	2451	O	PRO	B	443	79.442	119.348	174.008	1.00	107.52
35	2452	N	GLU	B	444	78.391	118.073	175.529	1.00	79.76
	2453	CA	GLU	B	444	79.594	117.429	176.022	1.00	111.19
	2454	CB	GLU	B	444	79.710	117.589	177.542	1.00	148.56
	2455	CG	GLU	B	444	80.142	118.972	178.015	1.00	175.46
	2456	CD	GLU	B	444	79.828	119.211	179.486	1.00	159.46
40	2457	OE1	GLU	B	444	79.978	118.265	180.292	1.00	128.82
	2458	OE2	GLU	B	444	79.438	120.349	179.836	1.00	148.10
	2459	C	GLU	B	444	79.351	115.976	175.686	1.00	93.99
	2460	O	GLU	B	444	78.357	115.406	176.121	1.00	102.87
	2461	N	VAL	B	445	80.235	115.375	174.903	1.00	98.05
45	2462	CA	VAL	B	445	80.056	113.978	174.543	1.00	82.80
	2463	CB	VAL	B	445	79.787	113.845	173.042	1.00	75.64
	2464	CG1	VAL	B	445	80.696	114.770	172.266	1.00	56.15
	2465	CG2	VAL	B	445	79.983	112.403	172.620	1.00	100.09
	2466	C	VAL	B	445	81.230	113.081	174.936	1.00	52.47
50	2467	O	VAL	B	445	82.385	113.474	174.820	1.00	84.33
	2468	N	TYR	B	446	80.917	111.877	175.406	1.00	58.93
	2469	CA	TYR	B	446	81.928	110.913	175.817	1.00	94.16
	2470	CB	TYR	B	446	82.051	110.897	177.344	1.00	114.12
	2471	CG	TYR	B	446	82.132	112.276	177.967	1.00	123.21
55	2472	CD1	TYR	B	446	81.042	112.826	178.628	1.00	107.03

	2473	CE1	TYR	B	446	81.091	114.111	179.161	1.00	140.23
	2474	CD2	TYR	B	446	83.288	113.048	177.854	1.00	175.76
	2475	CE2	TYR	B	446	83.347	114.338	178.384	1.00	166.71
	2476	CZ	TYR	B	446	82.242	114.861	179.034	1.00	148.92
5	2477	OH	TYR	B	446	82.281	116.137	179.545	1.00	163.80
	2478	C	TYR	B	446	81.515	109.532	175.325	1.00	98.27
	2479	O	TYR	B	446	80.467	109.032	175.715	1.00	94.14
	2480	N	ALA	B	447	82.337	108.917	174.476	1.00	102.60
	2481	CA	ALA	B	447	82.035	107.592	173.925	1.00	60.72
10	2482	CB	ALA	B	447	82.452	107.548	172.479	1.00	85.56
	2483	C	ALA	B	447	82.706	106.451	174.698	1.00	79.19
	2484	O	ALA	B	447	83.836	106.585	175.166	1.00	86.10
	2485	N	PHE	B	448	82.018	105.322	174.823	1.00	45.82
	2486	CA	PHE	B	448	82.569	104.190	175.560	1.00	98.07
15	2487	CB	PHE	B	448	81.848	104.064	176.905	1.00	113.90
	2488	CG	PHE	B	448	81.973	105.292	177.762	1.00	142.00
	2489	CD1	PHE	B	448	81.192	106.412	177.512	1.00	154.40
	2490	CD2	PHE	B	448	82.920	105.353	178.777	1.00	186.99
	2491	CE1	PHE	B	448	81.356	107.576	178.258	1.00	156.24
20	2492	CE2	PHE	B	448	83.091	106.511	179.529	1.00	185.02
	2493	CZ	PHE	B	448	82.309	107.625	179.268	1.00	183.09
	2494	C	PHE	B	448	82.528	102.867	174.795	1.00	87.01
	2495	O	PHE	B	448	82.229	102.854	173.608	1.00	104.18
	2496	N	ALA	B	449	82.843	101.761	175.468	1.00	79.78
25	2497	CA	ALA	B	449	82.846	100.458	174.814	1.00	40.21
	2498	CB	ALA	B	449	83.970	100.401	173.803	1.00	97.16
	2499	C	ALA	B	449	82.959	99.284	175.780	1.00	54.65
	2500	O	ALA	B	449	83.846	99.231	176.623	1.00	65.36
	2501	N	THR	B	450	82.061	98.325	175.619	1.00	48.81
30	2502	CA	THR	B	450	81.993	97.144	176.467	1.00	85.23
	2503	CB	THR	B	450	80.626	96.450	176.266	1.00	58.63
	2504	OG1	THR	B	450	79.578	97.340	176.657	1.00	98.59
	2505	CG2	THR	B	450	80.529	95.176	177.085	1.00	107.27
	2506	C	THR	B	450	83.088	96.099	176.252	1.00	86.98
35	2507	O	THR	B	450	83.677	96.015	175.182	1.00	115.23
	2508	N	PRO	B	451	83.398	95.317	177.298	1.00	82.22
	2509	CD	PRO	B	451	83.248	95.823	178.669	1.00	78.05
	2510	CA	PRO	B	451	84.401	94.247	177.274	1.00	102.30
	2511	CB	PRO	B	451	84.895	94.197	178.715	1.00	127.73
40	2512	CG	PRO	B	451	84.606	95.567	179.233	1.00	117.16
	2513	C	PRO	B	451	83.638	92.976	176.904	1.00	102.38
	2514	O	PRO	B	451	82.434	92.893	177.140	1.00	107.16
	2515	N	GLU	B	452	84.316	91.984	176.339	1.00	119.75
	2516	CA	GLU	B	452	83.619	90.760	175.950	1.00	135.04
45	2517	CB	GLU	B	452	84.588	89.759	175.301	1.00	160.10
	2518	CG	GLU	B	452	85.720	89.279	176.195	1.00	192.95
	2519	CD	GLU	B	452	86.553	88.193	175.536	1.00	193.27
	2520	OE1	GLU	B	452	85.996	87.113	175.242	1.00	173.50
	2521	OE2	GLU	B	452	87.762	88.420	175.311	1.00	191.58
50	2522	C	GLU	B	452	82.901	90.097	177.120	1.00	120.59
	2523	O	GLU	B	452	83.117	90.448	178.278	1.00	87.28
	2524	N	TRP	B	453	82.040	89.138	176.797	1.00	120.79
	2525	CA	TRP	B	453	81.274	88.403	177.793	1.00	141.89
	2526	CB	TRP	B	453	79.909	89.074	177.986	1.00	165.76
55	2527	CG	TRP	B	453	78.970	88.353	178.913	1.00	194.36

	2528	CD2	TRP	B	453	78.780	88.606	180.312	1.00	210.98
	2529	CE2	TRP	B	453	77.810	87.688	180.773	1.00	213.28
	2530	CE3	TRP	B	453	79.338	89.515	181.221	1.00	215.87
	2531	CD1	TRP	B	453	78.130	87.324	178.595	1.00	204.35
5	2532	NE1	TRP	B	453	77.429	86.920	179.705	1.00	205.41
	2533	CZ2	TRP	B	453	77.382	87.656	182.106	1.00	220.95
	2534	CZ3	TRP	B	453	78.913	89.483	182.547	1.00	216.68
	2535	CH2	TRP	B	453	77.945	88.557	182.975	1.00	222.83
	2536	C	TRP	B	453	81.111	86.952	177.340	1.00	151.58
10	2537	O	TRP	B	453	80.894	86.679	176.161	1.00	148.39
	2538	N	PRO	B	454	81.227	86.000	178.277	1.00	154.83
	2539	CD	PRO	B	454	81.493	86.244	179.707	1.00	142.37
	2540	CA	PRO	B	454	81.101	84.563	178.014	1.00	175.73
	2541	CB	PRO	B	454	80.922	83.982	179.410	1.00	177.55
15	2542	CG	PRO	B	454	81.817	84.854	180.224	1.00	168.66
	2543	C	PRO	B	454	79.962	84.171	177.075	1.00	189.74
	2544	O	PRO	B	454	79.983	83.092	176.485	1.00	208.45
	2545	N	GLY	B	455	78.971	85.045	176.945	1.00	196.85
	2546	CA	GLY	B	455	77.842	84.759	176.078	1.00	187.96
20	2547	C	GLY	B	455	78.211	84.739	174.607	1.00	180.32
	2548	O	GLY	B	455	77.762	83.871	173.859	1.00	192.44
	2549	N	SER	B	456	79.029	85.701	174.192	1.00	169.42
	2550	CA	SER	B	456	79.463	85.802	172.801	1.00	166.91
	2551	CB	SER	B	456	78.471	86.631	171.992	1.00	158.61
25	2552	OG	SER	B	456	78.452	87.968	172.457	1.00	140.70
	2553	C	SER	B	456	80.824	86.474	172.755	1.00	166.74
	2554	O	SER	B	456	81.092	87.397	173.523	1.00	173.32
	2555	N	ARG	B	457	81.677	86.022	171.844	1.00	174.22
	2556	CA	ARG	B	457	83.016	86.582	171.723	1.00	176.54
30	2557	CB	ARG	B	457	84.057	85.452	171.727	1.00	182.95
	2558	CG	ARG	B	457	83.970	84.538	172.946	1.00	199.86
	2559	CD	ARG	B	457	85.036	83.449	172.934	1.00	203.45
	2560	NE	ARG	B	457	84.881	82.538	174.067	1.00	215.80
	2561	CZ	ARG	B	457	85.704	81.529	174.339	1.00	205.75
35	2562	NH1	ARG	B	457	86.751	81.296	173.558	1.00	206.61
	2563	NH2	ARG	B	457	85.479	80.751	175.391	1.00	185.40
	2564	C	ARG	B	457	83.180	87.431	170.468	1.00	160.43
	2565	O	ARG	B	457	84.282	87.892	170.169	1.00	168.18
	2566	N	ASP	B	458	82.090	87.647	169.737	1.00	145.98
40	2567	CA	ASP	B	458	82.161	88.438	168.512	1.00	164.53
	2568	CB	ASP	B	458	82.048	87.527	167.289	1.00	187.11
	2569	CG	ASP	B	458	83.221	86.575	167.162	1.00	204.04
	2570	OD1	ASP	B	458	84.377	87.051	167.162	1.00	205.31
	2571	OD2	ASP	B	458	82.989	85.352	167.062	1.00	200.56
45	2572	C	ASP	B	458	81.118	89.543	168.419	1.00	166.34
	2573	O	ASP	B	458	80.827	90.043	167.329	1.00	100.86
	2574	N	LYS	B	459	80.561	89.920	169.566	1.00	179.43
	2575	CA	LYS	B	459	79.561	90.978	169.629	1.00	157.46
	2576	CB	LYS	B	459	78.155	90.385	169.808	1.00	170.13
50	2577	CG	LYS	B	459	77.680	89.492	168.663	1.00	195.45
	2578	CD	LYS	B	459	76.254	88.985	168.892	1.00	180.52
	2579	CE	LYS	B	459	75.783	88.106	167.737	1.00	168.06
	2580	NZ	LYS	B	459	74.380	87.632	167.911	1.00	140.21
	2581	C	LYS	B	459	79.886	91.894	170.805	1.00	156.35
55	2582	O	LYS	B	459	79.922	91.450	171.953	1.00	165.29

	2583	N	ARG	B	460	80.140	93.167	170.515	1.00	147.60
	2584	CA	ARG	B	460	80.444	94.141	171.561	1.00	148.70
	2585	CB	ARG	B	460	81.942	94.468	171.566	1.00	116.00
	2586	CG	ARG	B	460	82.793	93.307	172.076	1.00	133.11
5	2587	CD	ARG	B	460	84.209	93.727	172.454	1.00	145.86
	2588	NE	ARG	B	460	84.924	92.645	173.130	1.00	154.57
	2589	CZ	ARG	B	460	86.106	92.776	173.728	1.00	176.49
	2590	NH1	ARG	B	460	86.723	93.949	173.741	1.00	156.00
	2591	NH2	ARG	B	460	86.673	91.733	174.320	1.00	195.46
10	2592	C	ARG	B	460	79.595	95.410	171.423	1.00	134.14
	2593	O	ARG	B	460	79.384	95.915	170.320	1.00	108.53
	2594	N	THR	B	461	79.124	95.914	172.562	1.00	97.76
	2595	CA	THR	B	461	78.240	97.078	172.631	1.00	80.21
	2596	CB	THR	B	461	77.224	96.860	173.750	1.00	88.28
15	2597	OG1	THR	B	461	76.775	95.499	173.711	1.00	112.83
	2598	CG2	THR	B	461	76.037	97.804	173.597	1.00	61.89
	2599	C	THR	B	461	78.845	98.467	172.849	1.00	76.50
	2600	O	THR	B	461	79.691	98.647	173.719	1.00	62.71
	2601	N	LEU	B	462	78.385	99.453	172.079	1.00	66.18
20	2602	CA	LEU	B	462	78.869	100.827	172.229	1.00	94.33
	2603	CB	LEU	B	462	79.268	101.446	170.885	1.00	67.03
	2604	CG	LEU	B	462	80.510	100.946	170.147	1.00	85.83
	2605	CD1	LEU	B	462	81.004	102.049	169.214	1.00	60.23
	2606	CD2	LEU	B	462	81.594	100.578	171.134	1.00	69.11
25	2607	C	LEU	B	462	77.811	101.721	172.867	1.00	93.33
	2608	O	LEU	B	462	76.612	101.466	172.742	1.00	137.10
	2609	N	ALA	B	463	78.267	102.777	173.538	1.00	84.75
	2610	CA	ALA	B	463	77.385	103.730	174.207	1.00	57.78
	2611	CB	ALA	B	463	77.231	103.369	175.655	1.00	67.02
30	2612	C	ALA	B	463	77.982	105.115	174.089	1.00	65.49
	2613	O	ALA	B	463	79.197	105.283	174.138	1.00	79.68
	2614	N	CYS	B	464	77.127	106.114	173.950	1.00	77.94
	2615	CA	CYS	B	464	77.599	107.476	173.795	1.00	76.01
	2616	C	CYS	B	464	76.707	108.413	174.573	1.00	97.04
35	2617	O	CYS	B	464	75.511	108.494	174.317	1.00	118.25
	2618	CB	CYS	B	464	77.580	107.839	172.322	1.00	48.71
	2619	SG	CYS	B	464	78.259	109.457	171.871	1.00	108.42
	2620	N	LEU	B	465	77.300	109.120	175.526	1.00	104.12
	2621	CA	LEU	B	465	76.568	110.055	176.368	1.00	83.50
40	2622	CB	LEU	B	465	76.945	109.819	177.827	1.00	57.15
	2623	CG	LEU	B	465	76.704	110.946	178.820	1.00	72.22
	2624	CD1	LEU	B	465	75.332	111.558	178.626	1.00	80.58
	2625	CD2	LEU	B	465	76.872	110.378	180.214	1.00	78.64
	2626	C	LEU	B	465	76.796	111.517	175.999	1.00	76.86
45	2627	O	LEU	B	465	77.918	111.999	175.967	1.00	62.37
	2628	N	ILE	B	466	75.713	112.220	175.726	1.00	63.57
	2629	CA	ILE	B	466	75.794	113.617	175.367	1.00	60.62
	2630	CB	ILE	B	466	75.174	113.839	173.997	1.00	81.07
	2631	CG2	ILE	B	466	75.447	115.266	173.508	1.00	60.00
50	2632	CG1	ILE	B	466	75.729	112.784	173.042	1.00	33.92
	2633	CD1	ILE	B	466	75.341	113.005	171.599	1.00	85.20
	2634	C	ILE	B	466	75.029	114.398	176.420	1.00	93.44
	2635	O	ILE	B	466	73.826	114.215	176.575	1.00	96.66
	2636	N	GLN	B	467	75.723	115.271	177.142	1.00	102.53
55	2637	CA	GLN	B	467	75.072	116.033	178.195	1.00	81.78

	2638	CB	GLN	B	467	75.418	115.422	179.552	1.00	45.68
	2639	CG	GLN	B	467	76.895	115.224	179.783	1.00	79.30
	2640	CD	GLN	B	467	77.217	114.845	181.222	1.00	113.12
	2641	OE1	GLN	B	467	76.587	113.958	181.809	1.00	73.47
5	2642	NE2	GLN	B	467	78.213	115.514	181.794	1.00	129.90
	2643	C	GLN	B	467	75.318	117.535	178.260	1.00	57.56
	2644	O	GLN	B	467	75.964	118.136	177.400	1.00	58.32
	2645	N	ASN	B	468	74.751	118.122	179.306	1.00	90.17
	2646	CA	ASN	B	468	74.855	119.537	179.600	1.00	80.28
10	2647	CB	ASN	B	468	76.182	119.806	180.295	1.00	100.04
	2648	CG	ASN	B	468	76.430	118.848	181.444	1.00	135.69
	2649	OD1	ASN	B	468	75.579	118.677	182.323	1.00	115.44
	2650	ND2	ASN	B	468	77.598	118.211	181.442	1.00	138.13
	2651	C	ASN	B	468	74.695	120.436	178.395	1.00	92.36
15	2652	O	ASN	B	468	75.553	121.266	178.104	1.00	115.17
	2653	N	PHE	B	469	73.582	120.273	177.696	1.00	53.18
	2654	CA	PHE	B	469	73.314	121.103	176.537	1.00	71.01
	2655	CB	PHE	B	469	73.459	120.295	175.246	1.00	56.66
	2656	CG	PHE	B	469	72.531	119.107	175.155	1.00	100.03
20	2657	CD1	PHE	B	469	71.424	119.130	174.306	1.00	45.65
	2658	CD2	PHE	B	469	72.781	117.952	175.895	1.00	97.64
	2659	CE1	PHE	B	469	70.593	118.026	174.192	1.00	97.74
	2660	CE2	PHE	B	469	71.946	116.838	175.785	1.00	35.93
	2661	CZ	PHE	B	469	70.855	116.877	174.934	1.00	100.21
25	2662	C	PHE	B	469	71.917	121.672	176.618	1.00	72.62
	2663	O	PHE	B	469	71.106	121.247	177.450	1.00	57.82
	2664	N	MET	B	470	71.650	122.640	175.748	1.00	28.09
	2665	CA	MET	B	470	70.344	123.287	175.681	1.00	59.88
	2666	CB	MET	B	470	70.018	123.983	177.000	1.00	109.60
30	2667	CG	MET	B	470	71.139	124.822	177.586	1.00	125.93
	2668	SD	MET	B	470	71.008	124.868	179.393	1.00	132.45
	2669	CE	MET	B	470	69.604	125.930	179.600	1.00	165.70
	2670	C	MET	B	470	70.355	124.265	174.524	1.00	62.44
	2671	O	MET	B	470	71.359	124.924	174.279	1.00	61.44
35	2672	N	PRO	B	471	69.224	124.398	173.803	1.00	78.95
	2673	CD	PRO	B	471	69.191	125.344	172.677	1.00	80.51
	2674	CA	PRO	B	471	67.936	123.696	173.918	1.00	80.70
	2675	CB	PRO	B	471	67.159	124.210	172.709	1.00	74.00
	2676	CG	PRO	B	471	67.714	125.581	172.516	1.00	99.60
40	2677	C	PRO	B	471	68.028	122.180	173.923	1.00	80.76
	2678	O	PRO	B	471	69.116	121.612	173.879	1.00	103.67
	2679	N	GLU	B	472	66.879	121.518	173.962	1.00	88.76
	2680	CA	GLU	B	472	66.873	120.070	173.975	1.00	85.51
	2681	CB	GLU	B	472	65.665	119.551	174.757	1.00	112.19
45	2682	CG	GLU	B	472	64.326	120.100	174.287	1.00	171.67
	2683	CD	GLU	B	472	63.145	119.321	174.848	1.00	191.16
	2684	OE1	GLU	B	472	63.088	119.123	176.083	1.00	177.52
	2685	OE2	GLU	B	472	62.272	118.908	174.053	1.00	195.05
	2686	C	GLU	B	472	66.878	119.472	172.575	1.00	108.68
50	2687	O	GLU	B	472	67.002	118.258	172.429	1.00	108.87
	2688	N	ASP	B	473	66.748	120.310	171.548	1.00	67.19
	2689	CA	ASP	B	473	66.747	119.812	170.168	1.00	94.32
	2690	CB	ASP	B	473	66.278	120.901	169.206	1.00	108.16
	2691	CG	ASP	B	473	64.829	121.247	169.396	1.00	130.25
55	2692	OD1	ASP	B	473	64.004	120.313	169.448	1.00	152.46

	2693	OD2	ASP	B	473	64.511	122.446	169.486	1.00	127.62
	2694	C	ASP	B	473	68.118	119.302	169.725	1.00	86.57
	2695	O	ASP	B	473	69.002	120.089	169.380	1.00	76.15
	2696	N	ILE	B	474	68.283	117.982	169.704	1.00	86.59
5	2697	CA	ILE	B	474	69.559	117.388	169.332	1.00	62.99
	2698	CB	ILE	B	474	70.315	116.903	170.597	1.00	70.94
	2699	CG2	ILE	B	474	69.789	115.557	171.052	1.00	49.54
	2700	CG1	ILE	B	474	71.798	116.740	170.301	1.00	79.49
	2701	CD1	ILE	B	474	72.587	116.274	171.507	1.00	78.48
10	2702	C	ILE	B	474	69.446	116.217	168.360	1.00	81.03
	2703	O	ILE	B	474	68.513	115.412	168.436	1.00	79.23
	2704	N	SER	B	475	70.410	116.134	167.448	1.00	80.57
	2705	CA	SER	B	475	70.478	115.057	166.464	1.00	72.68
	2706	CB	SER	B	475	70.451	115.624	165.044	1.00	48.43
15	2707	OG	SER	B	475	69.152	115.552	164.488	1.00	90.69
	2708	C	SER	B	475	71.758	114.239	166.657	1.00	52.82
	2709	O	SER	B	475	72.857	114.708	166.371	1.00	78.59
	2710	N	VAL	B	476	71.611	113.020	167.154	1.00	56.94
	2711	CA	VAL	B	476	72.746	112.127	167.364	1.00	46.67
20	2712	CB	VAL	B	476	72.522	111.246	168.605	1.00	59.60
	2713	CG1	VAL	B	476	73.590	110.197	168.732	1.00	49.38
	2714	CG2	VAL	B	476	72.520	112.094	169.816	1.00	76.03
	2715	C	VAL	B	476	72.884	111.219	166.133	1.00	66.33
	2716	O	VAL	B	476	71.938	111.062	165.354	1.00	113.57
25	2717	N	GLN	B	477	74.065	110.632	165.961	1.00	72.08
	2718	CA	GLN	B	477	74.340	109.725	164.850	1.00	86.67
	2719	CB	GLN	B	477	74.256	110.474	163.530	1.00	59.98
	2720	CG	GLN	B	477	75.039	111.750	163.500	1.00	52.42
	2721	CD	GLN	B	477	74.806	112.507	162.215	1.00	113.14
30	2722	OE1	GLN	B	477	73.664	112.831	161.874	1.00	115.80
	2723	NE2	GLN	B	477	75.884	112.792	161.487	1.00	104.02
	2724	C	GLN	B	477	75.712	109.077	164.987	1.00	71.96
	2725	O	GLN	B	477	76.433	109.318	165.946	1.00	72.78
	2726	N	TRP	B	478	76.071	108.231	164.038	1.00	74.54
35	2727	CA	TRP	B	478	77.371	107.594	164.114	1.00	91.24
	2728	CB	TRP	B	478	77.254	106.181	164.656	1.00	30.97
	2729	CG	TRP	B	478	76.687	106.064	166.023	1.00	64.60
	2730	CD2	TRP	B	478	77.409	105.759	167.220	1.00	55.53
	2731	CE2	TRP	B	478	76.461	105.528	168.231	1.00	51.61
40	2732	CE3	TRP	B	478	78.767	105.646	167.531	1.00	88.58
	2733	CD1	TRP	B	478	75.371	106.032	166.355	1.00	68.44
	2734	NE1	TRP	B	478	75.222	105.702	167.676	1.00	76.50
	2735	CZ2	TRP	B	478	76.824	105.184	169.534	1.00	99.88
	2736	CZ3	TRP	B	478	79.129	105.302	168.828	1.00	73.67
45	2737	CH2	TRP	B	478	78.159	105.074	169.812	1.00	68.61
	2738	C	TRP	B	478	78.063	107.529	162.771	1.00	73.34
	2739	O	TRP	B	478	77.417	107.546	161.726	1.00	112.30
	2740	N	LEU	B	479	79.387	107.450	162.811	1.00	54.55
	2741	CA	LEU	B	479	80.171	107.362	161.597	1.00	75.53
50	2742	CB	LEU	B	479	80.982	108.634	161.420	1.00	86.60
	2743	CG	LEU	B	479	80.135	109.894	161.606	1.00	64.71
	2744	CD1	LEU	B	479	81.024	111.119	161.500	1.00	143.30
	2745	CD2	LEU	B	479	79.031	109.939	160.564	1.00	91.15
	2746	C	LEU	B	479	81.081	106.160	161.743	1.00	90.65
55	2747	O	LEU	B	479	81.316	105.695	162.856	1.00	67.67

	2748	N	HIS	B	480	81.582	105.652	160.621	1.00	130.81
	2749	CA	HIS	B	480	82.460	104.487	160.635	1.00	114.42
	2750	CB	HIS	B	480	81.646	103.225	160.911	1.00	109.89
	2751	CG	HIS	B	480	82.423	101.954	160.772	1.00	101.08
5	2752	CD2	HIS	B	480	82.120	100.790	160.152	1.00	114.03
	2753	ND1	HIS	B	480	83.644	101.759	161.379	1.00	82.41
	2754	CE1	HIS	B	480	84.057	100.527	161.144	1.00	108.15
	2755	NE2	HIS	B	480	83.151	99.917	160.402	1.00	119.50
	2756	C	HIS	B	480	83.186	104.348	159.316	1.00	84.59
10	2757	O	HIS	B	480	82.657	103.811	158.351	1.00	86.39
	2758	N	ASN	B	481	84.406	104.846	159.275	1.00	93.11
	2759	CA	ASN	B	481	85.181	104.760	158.059	1.00	118.77
	2760	CB	ASN	B	481	85.276	103.302	157.612	1.00	96.52
	2761	CG	ASN	B	481	86.518	103.023	156.817	1.00	137.81
15	2762	OD1	ASN	B	481	86.812	101.876	156.498	1.00	143.19
	2763	ND2	ASN	B	481	87.262	104.075	156.488	1.00	162.07
	2764	C	ASN	B	481	84.527	105.608	156.973	1.00	70.50
	2765	O	ASN	B	481	84.388	105.183	155.836	1.00	95.06
	2766	N	GLU	B	482	84.126	106.814	157.345	1.00	75.74
20	2767	CA	GLU	B	482	83.512	107.746	156.415	1.00	123.11
	2768	CB	GLU	B	482	84.424	107.940	155.198	1.00	121.91
	2769	CG	GLU	B	482	85.873	108.306	155.542	1.00	142.86
	2770	CD	GLU	B	482	86.012	109.651	156.248	1.00	171.49
	2771	OE1	GLU	B	482	85.641	110.686	155.650	1.00	170.24
25	2772	OE2	GLU	B	482	86.497	109.672	157.401	1.00	170.99
	2773	C	GLU	B	482	82.130	107.277	155.969	1.00	104.98
	2774	O	GLU	B	482	81.647	107.661	154.902	1.00	66.15
	2775	N	VAL	B	483	81.490	106.457	156.795	1.00	66.23
	2776	CA	VAL	B	483	80.164	105.948	156.472	1.00	92.18
30	2777	CB	VAL	B	483	80.210	104.427	156.245	1.00	99.60
	2778	CG1	VAL	B	483	78.813	103.869	156.069	1.00	96.51
	2779	CG2	VAL	B	483	81.050	104.125	155.022	1.00	173.41
	2780	C	VAL	B	483	79.140	106.250	157.562	1.00	113.67
	2781	O	VAL	B	483	79.184	105.661	158.640	1.00	139.78
35	2782	N	GLN	B	484	78.214	107.164	157.276	1.00	105.77
	2783	CA	GLN	B	484	77.165	107.533	158.231	1.00	69.76
	2784	CB	GLN	B	484	76.416	108.768	157.735	1.00	107.20
	2785	CG	GLN	B	484	75.352	109.285	158.681	1.00	78.17
	2786	CD	GLN	B	484	74.564	110.423	158.077	1.00	122.38
40	2787	OE1	GLN	B	484	75.132	111.338	157.474	1.00	88.01
	2788	NE2	GLN	B	484	73.248	110.378	158.238	1.00	132.45
	2789	C	GLN	B	484	76.177	106.385	158.392	1.00	52.68
	2790	O	GLN	B	484	75.234	106.268	157.616	1.00	96.63
	2791	N	LEU	B	485	76.386	105.553	159.408	1.00	54.65
45	2792	CA	LEU	B	485	75.529	104.401	159.636	1.00	61.68
	2793	CB	LEU	B	485	75.859	103.754	160.976	1.00	56.33
	2794	CG	LEU	B	485	77.220	103.068	161.101	1.00	54.48
	2795	CD1	LEU	B	485	77.171	102.084	162.246	1.00	62.35
	2796	CD2	LEU	B	485	77.554	102.325	159.813	1.00	115.96
50	2797	C	LEU	B	485	74.025	104.629	159.534	1.00	77.38
	2798	O	LEU	B	485	73.537	105.746	159.679	1.00	81.23
	2799	N	PRO	B	486	73.271	103.551	159.266	1.00	73.49
	2800	CD	PRO	B	486	73.794	102.217	158.934	1.00	122.28
	2801	CA	PRO	B	486	71.819	103.570	159.127	1.00	82.90
55	2802	CB	PRO	B	486	71.492	102.137	158.712	1.00	119.65

	2803	CG	PRO	B	486	72.729	101.692	158.018	1.00	136.98
	2804	C	PRO	B	486	71.154	103.952	160.433	1.00	94.37
	2805	O	PRO	B	486	71.429	103.370	161.481	1.00	68.92
	2806	N	ASP	B	487	70.268	104.932	160.359	1.00	84.31
	2807	CA	ASP	B	487	69.560	105.398	161.533	1.00	88.88
	2808	CB	ASP	B	487	68.424	106.329	161.097	1.00	108.41
	2809	CG	ASP	B	487	68.070	107.347	162.155	1.00	154.62
	2810	OD1	ASP	B	487	67.549	106.946	163.217	1.00	160.64
	2811	OD2	ASP	B	487	68.322	108.549	161.926	1.00	168.53
	2812	C	ASP	B	487	69.014	104.240	162.374	1.00	63.64
	2813	O	ASP	B	487	69.085	104.269	163.596	1.00	90.99
	2814	N	ALA	B	488	68.492	103.210	161.721	1.00	64.28
	2815	CA	ALA	B	488	67.910	102.073	162.432	1.00	73.64
	2816	CB	ALA	B	488	67.073	101.232	161.463	1.00	116.29
	2817	C	ALA	B	488	68.921	101.189	163.143	1.00	75.09
	2818	O	ALA	B	488	68.563	100.164	163.722	1.00	61.17
	2819	N	ARG	B	489	70.180	101.599	163.122	1.00	47.46
	2820	CA	ARG	B	489	71.245	100.817	163.739	1.00	76.59
	2821	CB	ARG	B	489	72.562	101.088	163.014	1.00	92.18
	2822	CG	ARG	B	489	72.771	100.227	161.785	1.00	116.98
	2823	CD	ARG	B	489	73.469	98.935	162.162	1.00	101.72
	2824	NE	ARG	B	489	74.904	99.013	161.904	1.00	96.78
	2825	CZ	ARG	B	489	75.803	98.212	162.459	1.00	108.26
	2826	NH1	ARG	B	489	75.418	97.273	163.311	1.00	104.09
	2827	NH2	ARG	B	489	77.084	98.345	162.157	1.00	106.78
	2828	C	ARG	B	489	71.432	101.066	165.219	1.00	78.64
	2829	O	ARG	B	489	71.773	100.153	165.972	1.00	80.15
	2830	N	HIS	B	490	71.205	102.308	165.631	1.00	85.57
	2831	CA	HIS	B	490	71.377	102.703	167.023	1.00	79.08
	2832	CB	HIS	B	490	72.359	103.863	167.106	1.00	65.14
	2833	CG	HIS	B	490	71.883	105.094	166.405	1.00	51.35
	2834	CD2	HIS	B	490	70.847	105.924	166.669	1.00	81.18
	2835	ND1	HIS	B	490	72.493	105.592	165.276	1.00	77.41
	2836	CE1	HIS	B	490	71.855	106.678	164.874	1.00	76.90
	2837	NE2	HIS	B	490	70.852	106.901	165.703	1.00	118.70
	2838	C	HIS	B	490	70.086	103.134	167.690	1.00	75.63
	2839	O	HIS	B	490	69.136	103.545	167.028	1.00	82.18
	2840	N	SER	B	491	70.072	103.056	169.017	1.00	111.19
	2841	CA	SER	B	491	68.915	103.461	169.801	1.00	98.54
	2842	CB	SER	B	491	68.477	102.333	170.737	1.00	70.59
	2843	OG	SER	B	491	67.305	102.703	171.444	1.00	151.07
	2844	C	SER	B	491	69.295	104.683	170.624	1.00	91.58
	2845	O	SER	B	491	70.209	104.630	171.439	1.00	69.75
	2846	N	THR	B	492	68.600	105.790	170.402	1.00	103.48
	2847	CA	THR	B	492	68.874	107.011	171.149	1.00	84.76
	2848	CB	THR	B	492	69.182	108.171	170.208	1.00	96.92
	2849	OG1	THR	B	492	70.431	107.927	169.553	1.00	98.55
	2850	CG2	THR	B	492	69.260	109.473	170.978	1.00	89.03
	2851	C	THR	B	492	67.666	107.370	172.002	1.00	95.54
	2852	O	THR	B	492	66.532	107.352	171.523	1.00	110.69
	2853	N	THR	B	493	67.907	107.702	173.266	1.00	65.05
	2854	CA	THR	B	493	66.809	108.036	174.159	1.00	70.59
	2855	CB	THR	B	493	67.188	107.882	175.635	1.00	74.90
	2856	OG1	THR	B	493	68.008	108.984	176.019	1.00	55.82
	2857	CG2	THR	B	493	67.929	106.576	175.874	1.00	80.05

	2858	C	THR	B	493	66.315	109.457	173.978	1.00	81.61
	2859	O	THR	B	493	66.765	110.190	173.102	1.00	64.79
	2860	N	GLN	B	494	65.365	109.834	174.820	1.00	97.42
	2861	CA	GLN	B	494	64.806	111.166	174.769	1.00	90.31
	2862	CB	GLN	B	494	63.296	111.115	175.033	1.00	108.14
	2863	CG	GLN	B	494	62.486	110.334	174.005	1.00	116.36
	2864	CD	GLN	B	494	62.660	110.860	172.584	1.00	154.38
	2865	OE1	GLN	B	494	62.652	112.070	172.350	1.00	129.72
	2866	NE2	GLN	B	494	62.804	109.947	171.627	1.00	166.89
	2867	C	GLN	B	494	65.498	112.012	175.833	1.00	107.40
	2868	O	GLN	B	494	65.869	111.509	176.900	1.00	110.85
	2869	N	PRO	B	495	65.697	113.309	175.547	1.00	81.82
	2870	CD	PRO	B	495	65.416	113.972	174.261	1.00	69.03
	2871	CA	PRO	B	495	66.342	114.240	176.470	1.00	65.90
	2872	CB	PRO	B	495	66.109	115.583	175.802	1.00	63.09
	2873	CG	PRO	B	495	66.235	115.239	174.363	1.00	52.88
	2874	C	PRO	B	495	65.742	114.186	177.867	1.00	75.89
	2875	O	PRO	B	495	64.558	113.914	178.039	1.00	107.23
	2876	N	ARG	B	496	66.580	114.437	178.862	1.00	112.34
	2877	CA	ARG	B	496	66.166	114.445	180.257	1.00	123.31
	2878	CB	ARG	B	496	66.434	113.080	180.902	1.00	145.69
	2879	CG	ARG	B	496	65.366	112.031	180.599	1.00	159.05
	2880	CD	ARG	B	496	65.774	110.643	181.091	1.00	178.53
	2881	NE	ARG	B	496	64.643	109.715	181.137	1.00	209.19
	2882	CZ	ARG	B	496	63.715	109.707	182.092	1.00	207.25
	2883	NH1	ARG	B	496	63.779	110.578	183.092	1.00	201.73
	2884	NH2	ARG	B	496	62.717	108.832	182.044	1.00	194.79
	2885	C	ARG	B	496	66.963	115.549	180.944	1.00	134.53
	2886	O	ARG	B	496	68.121	115.798	180.597	1.00	112.03
	2887	N	LYS	B	497	66.341	116.220	181.907	1.00	136.67
	2888	CA	LYS	B	497	66.999	117.318	182.601	1.00	99.35
	2889	CB	LYS	B	497	65.955	118.224	183.252	1.00	115.41
	2890	CG	LYS	B	497	64.939	118.793	182.278	1.00	150.70
	2891	CD	LYS	B	497	63.952	119.718	182.976	1.00	164.39
	2892	CE	LYS	B	497	62.907	120.251	182.003	1.00	162.23
	2893	NZ	LYS	B	497	61.957	121.204	182.648	1.00	146.92
	2894	C	LYS	B	497	68.005	116.876	183.649	1.00	102.60
	2895	O	LYS	B	497	67.966	115.743	184.129	1.00	95.44
	2896	N	THR	B	498	68.906	117.792	183.993	1.00	121.19
	2897	CA	THR	B	498	69.940	117.543	184.989	1.00	137.86
	2898	CB	THR	B	498	71.330	117.388	184.326	1.00	127.01
	2899	OG1	THR	B	498	71.571	118.479	183.426	1.00	102.85
	2900	CG2	THR	B	498	71.398	116.094	183.555	1.00	140.90
	2901	C	THR	B	498	69.995	118.681	186.008	1.00	162.55
	2902	O	THR	B	498	69.507	119.788	185.754	1.00	135.49
	2903	N	LYS	B	499	70.589	118.405	187.164	1.00	151.73
	2904	CA	LYS	B	499	70.701	119.410	188.212	1.00	168.61
	2905	CB	LYS	B	499	71.167	118.755	189.520	1.00	183.90
	2906	CG	LYS	B	499	70.993	119.632	190.759	1.00	193.98
	2907	CD	LYS	B	499	71.224	118.849	192.051	1.00	178.03
	2908	CE	LYS	B	499	70.926	119.704	193.283	1.00	168.01
	2909	NZ	LYS	B	499	71.031	118.937	194.562	1.00	137.47
	2910	C	LYS	B	499	71.677	120.509	187.780	1.00	173.90
	2911	O	LYS	B	499	72.200	121.257	188.606	1.00	189.46
	2912	N	GLY	B	500	71.910	120.597	186.473	1.00	172.18

	2913	CA	GLY	B	500	72.811	121.601	185.936	1.00	169.02
	2914	C	GLY	B	500	72.141	122.406	184.837	1.00	176.17
	2915	O	GLY	B	500	72.813	122.959	183.965	1.00	182.74
	2916	N	SER	B	501	70.810	122.456	184.884	1.00	151.02
5	2917	CA	SER	B	501	69.989	123.189	183.919	1.00	147.04
	2918	CB	SER	B	501	70.242	124.698	184.044	1.00	152.23
	2919	OG	SER	B	501	71.556	125.048	183.642	1.00	182.63
	2920	C	SER	B	501	70.164	122.762	182.458	1.00	151.49
	2921	O	SER	B	501	69.620	123.395	181.549	1.00	133.52
10	2922	N	GLY	B	502	70.916	121.691	182.230	1.00	142.82
	2923	CA	GLY	B	502	71.116	121.218	180.873	1.00	95.52
	2924	C	GLY	B	502	70.507	119.842	180.705	1.00	118.00
	2925	O	GLY	B	502	70.114	119.219	181.689	1.00	106.89
	2926	N	PHE	B	503	70.421	119.358	179.469	1.00	108.44
15	2927	CA	PHE	B	503	69.850	118.035	179.231	1.00	93.09
	2928	CB	PHE	B	503	68.868	118.051	178.071	1.00	70.27
	2929	CG	PHE	B	503	67.813	119.092	178.173	1.00	78.42
	2930	CD1	PHE	B	503	68.002	120.346	177.604	1.00	94.67
	2931	CD2	PHE	B	503	66.605	118.803	178.782	1.00	58.13
20	2932	CE1	PHE	B	503	66.990	121.300	177.635	1.00	98.84
	2933	CE2	PHE	B	503	65.587	119.749	178.819	1.00	113.56
	2934	CZ	PHE	B	503	65.779	121.001	178.243	1.00	112.26
	2935	C	PHE	B	503	70.909	116.995	178.911	1.00	91.24
	2936	O	PHE	B	503	72.074	117.326	178.682	1.00	63.55
25	2937	N	PHE	B	504	70.474	115.737	178.867	1.00	71.28
	2938	CA	PHE	B	504	71.354	114.618	178.578	1.00	66.45
	2939	CB	PHE	B	504	71.965	114.102	179.879	1.00	66.76
	2940	CG	PHE	B	504	71.102	113.121	180.617	1.00	55.05
	2941	CD1	PHE	B	504	71.121	111.776	180.286	1.00	75.50
30	2942	CD2	PHE	B	504	70.308	113.532	181.672	1.00	92.55
	2943	CE1	PHE	B	504	70.367	110.853	181.003	1.00	87.60
	2944	CE2	PHE	B	504	69.551	112.614	182.394	1.00	119.03
	2945	CZ	PHE	B	504	69.583	111.271	182.057	1.00	113.46
	2946	C	PHE	B	504	70.627	113.477	177.864	1.00	71.40
35	2947	O	PHE	B	504	69.534	113.078	178.262	1.00	98.42
	2948	N	VAL	B	505	71.240	112.949	176.809	1.00	93.14
	2949	CA	VAL	B	505	70.652	111.844	176.061	1.00	85.70
	2950	CB	VAL	B	505	70.169	112.299	174.672	1.00	64.09
	2951	CG1	VAL	B	505	71.345	112.676	173.807	1.00	32.54
40	2952	CG2	VAL	B	505	69.357	111.195	174.029	1.00	103.96
	2953	C	VAL	B	505	71.669	110.722	175.888	1.00	58.13
	2954	O	VAL	B	505	72.859	110.973	175.798	1.00	86.55
	2955	N	PHE	B	506	71.187	109.487	175.841	1.00	81.98
	2956	CA	PHE	B	506	72.035	108.311	175.685	1.00	63.87
45	2957	CB	PHE	B	506	71.733	107.331	176.792	1.00	50.64
	2958	CG	PHE	B	506	72.585	107.497	178.006	1.00	61.69
	2959	CD1	PHE	B	506	72.100	107.129	179.255	1.00	87.69
	2960	CD2	PHE	B	506	73.900	107.921	177.902	1.00	101.17
	2961	CE1	PHE	B	506	72.904	107.168	180.385	1.00	55.65
50	2962	CE2	PHE	B	506	74.721	107.965	179.032	1.00	102.15
	2963	CZ	PHE	B	506	74.218	107.584	180.275	1.00	83.88
	2964	C	PHE	B	506	71.816	107.605	174.357	1.00	71.24
	2965	O	PHE	B	506	70.699	107.567	173.845	1.00	133.97
	2966	N	SER	B	507	72.883	107.036	173.803	1.00	84.07
55	2967	CA	SER	B	507	72.801	106.312	172.533	1.00	76.16

	2968	CB	SER	B	507	73.454	107.090	171.405	1.00	27.10
	2969	OG	SER	B	507	73.355	106.340	170.220	1.00	58.51
	2970	C	SER	B	507	73.480	104.962	172.635	1.00	57.27
	2971	O	SER	B	507	74.493	104.821	173.310	1.00	52.02
5	2972	N	ARG	B	508	72.924	103.967	171.958	1.00	51.27
	2973	CA	ARG	B	508	73.476	102.616	172.002	1.00	53.55
	2974	CB	ARG	B	508	72.623	101.735	172.911	1.00	44.14
	2975	CG	ARG	B	508	72.985	100.277	172.923	1.00	46.22
	2976	CD	ARG	B	508	72.144	99.540	173.949	1.00	70.79
10	2977	NE	ARG	B	508	72.340	98.093	173.925	1.00	49.24
	2978	CZ	ARG	B	508	71.855	97.291	172.984	1.00	103.44
	2979	NH1	ARG	B	508	71.147	97.796	171.984	1.00	133.71
	2980	NH2	ARG	B	508	72.064	95.983	173.054	1.00	124.77
	2981	C	ARG	B	508	73.541	102.032	170.601	1.00	62.86
15	2982	O	ARG	B	508	72.555	102.020	169.864	1.00	86.63
	2983	N	LEU	B	509	74.718	101.531	170.248	1.00	101.57
	2984	CA	LEU	B	509	74.962	100.979	168.925	1.00	91.96
	2985	CB	LEU	B	509	75.820	101.966	168.140	1.00	57.86
	2986	CG	LEU	B	509	76.358	101.480	166.804	1.00	69.57
20	2987	CD1	LEU	B	509	75.215	100.940	165.972	1.00	115.82
	2988	CD2	LEU	B	509	77.045	102.618	166.093	1.00	47.22
	2989	C	LEU	B	509	75.656	99.623	168.930	1.00	72.22
	2990	O	LEU	B	509	76.871	99.577	168.926	1.00	65.45
	2991	N	GLU	B	510	74.902	98.526	168.928	1.00	103.54
25	2992	CA	GLU	B	510	75.513	97.191	168.921	1.00	79.97
	2993	CB	GLU	B	510	74.427	96.107	168.847	1.00	105.98
	2994	CG	GLU	B	510	73.491	96.056	170.061	1.00	124.66
	2995	CD	GLU	B	510	72.349	95.050	169.905	1.00	156.13
	2996	OE1	GLU	B	510	71.488	95.247	169.018	1.00	161.88
30	2997	OE2	GLU	B	510	72.309	94.061	170.673	1.00	131.37
	2998	C	GLU	B	510	76.445	97.095	167.708	1.00	100.86
	2999	O	GLU	B	510	76.171	97.705	166.671	1.00	97.53
	3000	N	VAL	B	511	77.540	96.339	167.834	1.00	86.41
	3001	CA	VAL	B	511	78.512	96.196	166.741	1.00	113.22
35	3002	CB	VAL	B	511	79.763	97.091	166.993	1.00	29.35
	3003	CG1	VAL	B	511	80.823	96.827	165.953	1.00	119.74
	3004	CG2	VAL	B	511	79.373	98.544	166.915	1.00	108.86
	3005	C	VAL	B	511	78.981	94.760	166.461	1.00	152.83
	3006	O	VAL	B	511	78.941	93.899	167.343	1.00	151.08
40	3007	N	THR	B	512	79.428	94.522	165.225	1.00	167.98
	3008	CA	THR	B	512	79.908	93.212	164.786	1.00	153.93
	3009	CB	THR	B	512	79.252	92.806	163.446	1.00	164.28
	3010	OG1	THR	B	512	77.826	92.831	163.583	1.00	167.99
	3011	CG2	THR	B	512	79.691	91.403	163.034	1.00	183.03
45	3012	C	THR	B	512	81.427	93.180	164.604	1.00	134.07
	3013	O	THR	B	512	82.018	94.132	164.093	1.00	85.13
	3014	N	ARG	B	513	82.042	92.071	165.017	1.00	128.25
	3015	CA	ARG	B	513	83.488	91.879	164.910	1.00	132.09
	3016	CB	ARG	B	513	83.853	90.401	165.116	1.00	158.22
50	3017	CG	ARG	B	513	85.357	90.120	165.061	1.00	185.92
	3018	CD	ARG	B	513	85.684	88.632	165.174	1.00	210.68
	3019	NE	ARG	B	513	87.125	88.379	165.106	1.00	235.05
	3020	CZ	ARG	B	513	87.683	87.170	165.129	1.00	237.14
	3021	NH1	ARG	B	513	86.926	86.085	165.219	1.00	231.50
55	3022	NH2	ARG	B	513	89.003	87.045	165.060	1.00	226.13

	3023	C	ARG	B	513	84.028	92.345	163.566	1.00	119.35
	3024	O	ARG	B	513	84.945	93.157	163.504	1.00	73.78
	3025	N	ALA	B	514	83.450	91.824	162.492	1.00	114.41
	3026	CA	ALA	B	514	83.868	92.174	161.147	1.00	105.99
5	3027	CB	ALA	B	514	82.798	91.766	160.171	1.00	110.57
	3028	C	ALA	B	514	84.167	93.657	160.992	1.00	106.98
	3029	O	ALA	B	514	85.169	94.038	160.389	1.00	114.61
	3030	N	GLU	B	515	83.303	94.493	161.550	1.00	107.80
	3031	CA	GLU	B	515	83.461	95.936	161.440	1.00	100.76
10	3032	CB	GLU	B	515	82.162	96.623	161.855	1.00	61.09
	3033	CG	GLU	B	515	81.038	96.378	160.880	1.00	142.67
	3034	CD	GLU	B	515	79.733	96.989	161.327	1.00	158.22
	3035	OE1	GLU	B	515	79.234	96.590	162.401	1.00	121.42
	3036	OE2	GLU	B	515	79.210	97.862	160.600	1.00	163.79
15	3037	C	GLU	B	515	84.637	96.589	162.164	1.00	105.34
	3038	O	GLU	B	515	85.189	97.567	161.664	1.00	78.08
	3039	N	TRP	B	516	85.034	96.082	163.327	1.00	77.37
	3040	CA	TRP	B	516	86.146	96.723	164.007	1.00	80.12
	3041	CB	TRP	B	516	86.035	96.570	165.523	1.00	104.80
20	3042	CG	TRP	B	516	86.442	95.275	166.113	1.00	71.05
	3043	CD2	TRP	B	516	85.591	94.349	166.786	1.00	78.16
	3044	CE2	TRP	B	516	86.411	93.335	167.314	1.00	93.47
	3045	CE3	TRP	B	516	84.211	94.281	166.999	1.00	89.55
	3046	CD1	TRP	B	516	87.708	94.795	166.243	1.00	118.89
25	3047	NE1	TRP	B	516	87.702	93.630	166.968	1.00	138.68
	3048	CZ2	TRP	B	516	85.896	92.262	168.043	1.00	130.46
	3049	CZ3	TRP	B	516	83.698	93.218	167.722	1.00	72.54
	3050	CH2	TRP	B	516	84.539	92.222	168.236	1.00	115.85
	3051	C	TRP	B	516	87.493	96.250	163.505	1.00	126.19
30	3052	O	TRP	B	516	88.524	96.836	163.833	1.00	155.29
	3053	N	GLU	B	517	87.484	95.191	162.703	1.00	127.20
	3054	CA	GLU	B	517	88.715	94.681	162.120	1.00	102.94
	3055	CB	GLU	B	517	88.586	93.193	161.804	1.00	124.17
	3056	CG	GLU	B	517	88.437	92.331	163.045	1.00	150.03
35	3057	CD	GLU	B	517	88.603	90.854	162.756	1.00	194.54
	3058	OE1	GLU	B	517	87.847	90.322	161.915	1.00	209.80
	3059	OE2	GLU	B	517	89.490	90.226	163.373	1.00	178.99
	3060	C	GLU	B	517	88.923	95.495	160.848	1.00	118.06
	3061	O	GLU	B	517	90.047	95.697	160.396	1.00	141.82
40	3062	N	GLN	B	518	87.817	95.976	160.289	1.00	96.99
	3063	CA	GLN	B	518	87.840	96.803	159.093	1.00	108.10
	3064	CB	GLN	B	518	86.407	97.051	158.611	1.00	144.13
	3065	CG	GLN	B	518	86.285	97.795	157.287	1.00	173.67
	3066	CD	GLN	B	518	84.834	98.105	156.921	1.00	166.01
45	3067	OE1	GLN	B	518	83.989	97.206	156.851	1.00	119.41
	3068	NE2	GLN	B	518	84.544	99.382	156.686	1.00	143.37
	3069	C	GLN	B	518	88.500	98.116	159.504	1.00	120.74
	3070	O	GLN	B	518	89.196	98.743	158.710	1.00	92.65
	3071	N	LYS	B	519	88.260	98.509	160.758	1.00	130.00
50	3072	CA	LYS	B	519	88.818	99.719	161.375	1.00	130.50
	3073	CB	LYS	B	519	88.367	100.990	160.643	1.00	69.93
	3074	CG	LYS	B	519	89.179	102.223	161.053	1.00	87.64
	3075	CD	LYS	B	519	89.180	103.305	159.981	1.00	120.11
	3076	CE	LYS	B	519	90.255	104.358	160.255	1.00	120.69
55	3077	NZ	LYS	B	519	90.332	105.388	159.175	1.00	139.23

	3078	C	LYS	B	519	88.370	99.789	162.835	1.00	113.46
	3079	O	LYS	B	519	87.399	99.145	163.209	1.00	100.53
	3080	N	ASP	B	520	89.086	100.555	163.656	1.00	141.80
	3081	CA	ASP	B	520	88.752	100.712	165.075	1.00	91.69
5	3082	CB	ASP	B	520	90.013	100.687	165.939	1.00	139.47
	3083	CG	ASP	B	520	90.474	99.285	166.259	1.00	176.31
	3084	OD1	ASP	B	520	89.710	98.566	166.935	1.00	155.37
	3085	OD2	ASP	B	520	91.593	98.907	165.843	1.00	179.10
	3086	C	ASP	B	520	88.026	102.029	165.323	1.00	88.08
10	3087	O	ASP	B	520	87.179	102.115	166.201	1.00	108.19
	3088	N	GLU	B	521	88.367	103.055	164.552	1.00	111.16
	3089	CA	GLU	B	521	87.745	104.369	164.690	1.00	96.48
	3090	CB	GLU	B	521	88.335	105.364	163.686	1.00	137.30
	3091	CG	GLU	B	521	89.404	106.294	164.229	1.00	154.75
15	3092	CD	GLU	B	521	89.685	107.446	163.278	1.00	162.73
	3093	OE1	GLU	B	521	88.761	108.254	163.051	1.00	123.78
	3094	OE2	GLU	B	521	90.818	107.542	162.754	1.00	170.68
	3095	C	GLU	B	521	86.236	104.373	164.495	1.00	94.12
	3096	O	GLU	B	521	85.750	104.213	163.377	1.00	98.75
20	3097	N	PHE	B	522	85.506	104.574	165.588	1.00	125.98
	3098	CA	PHE	B	522	84.052	104.669	165.563	1.00	73.40
	3099	CB	PHE	B	522	83.424	103.654	166.495	1.00	46.93
	3100	CG	PHE	B	522	83.252	102.307	165.892	1.00	88.24
	3101	CD1	PHE	B	522	84.291	101.701	165.210	1.00	107.06
25	3102	CD2	PHE	B	522	82.051	101.625	166.026	1.00	126.15
	3103	CE1	PHE	B	522	84.137	100.430	164.671	1.00	144.12
	3104	CE2	PHE	B	522	81.887	100.353	165.491	1.00	86.55
	3105	CZ	PHE	B	522	82.929	99.756	164.814	1.00	98.88
	3106	C	PHE	B	522	83.737	106.065	166.062	1.00	85.06
30	3107	O	PHE	B	522	84.219	106.486	167.113	1.00	76.66
	3108	N	ILE	B	523	82.937	106.797	165.313	1.00	64.62
	3109	CA	ILE	B	523	82.619	108.140	165.731	1.00	93.86
	3110	CB	ILE	B	523	83.006	109.136	164.638	1.00	62.16
	3111	CG2	ILE	B	523	82.726	110.554	165.093	1.00	77.13
35	3112	CG1	ILE	B	523	84.483	108.963	164.309	1.00	68.68
	3113	CD1	ILE	B	523	85.004	109.946	163.268	1.00	144.70
	3114	C	ILE	B	523	81.152	108.304	166.076	1.00	89.50
	3115	O	ILE	B	523	80.276	107.800	165.371	1.00	97.40
	3116	N	CYS	B	524	80.903	108.998	167.183	1.00	89.54
40	3117	CA	CYS	B	524	79.551	109.286	167.642	1.00	88.30
	3118	C	CYS	B	524	79.358	110.792	167.558	1.00	53.16
	3119	O	CYS	B	524	79.589	111.496	168.514	1.00	59.51
	3120	CB	CYS	B	524	79.363	108.835	169.082	1.00	70.18
	3121	SG	CYS	B	524	77.896	109.575	169.868	1.00	102.40
45	3122	N	ARG	B	525	78.939	111.272	166.397	1.00	85.33
	3123	CA	ARG	B	525	78.740	112.694	166.166	1.00	42.18
	3124	CB	ARG	B	525	78.613	112.956	164.664	1.00	51.31
	3125	CG	ARG	B	525	78.750	114.395	164.270	1.00	55.59
	3126	CD	ARG	B	525	79.294	114.553	162.852	1.00	75.11
50	3127	NE	ARG	B	525	78.328	114.264	161.795	1.00	77.64
	3128	CZ	ARG	B	525	78.518	114.587	160.517	1.00	147.54
	3129	NH1	ARG	B	525	79.633	115.211	160.143	1.00	139.91
	3130	NH2	ARG	B	525	77.598	114.280	159.610	1.00	128.34
	3131	C	ARG	B	525	77.501	113.197	166.880	1.00	81.14
55	3132	O	ARG	B	525	76.714	112.411	167.406	1.00	77.17

	3133	N	ALA	B	526	77.344	114.517	166.897	1.00	86.44
	3134	CA	ALA	B	526	76.209	115.177	167.538	1.00	64.44
	3135	CB	ALA	B	526	76.469	115.358	169.025	1.00	40.12
	3136	C	ALA	B	526	76.003	116.527	166.881	1.00	64.81
5	3137	O	ALA	B	526	76.957	117.256	166.609	1.00	75.52
	3138	N	VAL	B	527	74.753	116.858	166.616	1.00	45.76
	3139	CA	VAL	B	527	74.446	118.123	165.984	1.00	48.87
	3140	CB	VAL	B	527	73.702	117.900	164.683	1.00	72.30
	3141	CG1	VAL	B	527	73.434	119.222	164.005	1.00	65.22
10	3142	CG2	VAL	B	527	74.512	116.984	163.798	1.00	69.67
	3143	C	VAL	B	527	73.583	118.949	166.912	1.00	62.63
	3144	O	VAL	B	527	72.494	118.525	167.296	1.00	107.55
	3145	N	HIS	B	528	74.075	120.123	167.290	1.00	88.39
	3146	CA	HIS	B	528	73.324	121.009	168.177	1.00	72.81
15	3147	CB	HIS	B	528	73.883	120.954	169.599	1.00	43.78
	3148	CG	HIS	B	528	73.000	121.603	170.619	1.00	68.69
	3149	CD2	HIS	B	528	72.544	122.873	170.730	1.00	102.41
	3150	ND1	HIS	B	528	72.530	120.932	171.727	1.00	114.24
	3151	CE1	HIS	B	528	71.828	121.761	172.479	1.00	111.59
20	3152	NE2	HIS	B	528	71.822	122.946	171.896	1.00	127.17
	3153	C	HIS	B	528	73.405	122.421	167.644	1.00	69.99
	3154	O	HIS	B	528	74.322	122.745	166.877	1.00	80.61
	3155	N	GLU	B	529	72.439	123.246	168.040	1.00	80.81
	3156	CA	GLU	B	529	72.388	124.630	167.603	1.00	110.94
25	3157	CB	GLU	B	529	71.056	125.236	168.007	1.00	143.10
	3158	CG	GLU	B	529	70.885	126.632	167.550	1.00	190.23
	3159	CD	GLU	B	529	69.576	127.233	168.045	1.00	209.79
	3160	OE1	GLU	B	529	69.275	128.356	168.100	1.00	211.79
	3161	OE2	GLU	B	529	68.633	126.689	168.465	1.00	204.23
30	3162	C	GLU	B	529	73.552	125.453	168.173	1.00	115.08
	3163	O	GLU	B	529	73.915	126.492	167.625	1.00	93.09
	3164	N	ALA	B	530	74.184	124.942	169.228	1.00	104.56
	3165	CA	ALA	B	530	75.301	125.633	169.882	1.00	119.10
	3166	CB	ALA	B	530	75.312	125.312	171.383	1.00	102.81
35	3167	C	ALA	B	530	76.657	125.298	169.285	1.00	143.44
	3168	O	ALA	B	530	77.105	125.948	168.341	1.00	167.11
	3169	N	ALA	B	531	77.296	124.287	169.868	1.00	133.04
	3170	CA	ALA	B	531	78.608	123.796	169.457	1.00	161.80
	3171	CB	ALA	B	531	78.530	122.299	169.233	1.00	131.50
40	3172	C	ALA	B	531	79.240	124.461	168.235	1.00	183.35
	3173	O	ALA	B	531	78.602	124.634	167.193	1.00	180.45
	3174	N	SER	B	532	80.513	124.816	168.369	1.00	186.13
	3175	CA	SER	B	532	81.245	125.437	167.279	1.00	159.85
	3176	CB	SER	B	532	81.945	126.707	167.764	1.00	149.12
45	3177	OG	SER	B	532	81.012	127.751	167.971	1.00	131.01
	3178	C	SER	B	532	82.270	124.459	166.721	1.00	143.48
	3179	O	SER	B	532	82.606	123.460	167.359	1.00	131.10
	3180	N	PRO	B	533	82.789	124.741	165.522	1.00	133.12
	3181	CD	PRO	B	533	84.018	124.105	165.014	1.00	145.42
50	3182	CA	PRO	B	533	82.446	125.915	164.718	1.00	114.44
	3183	CB	PRO	B	533	83.793	126.336	164.170	1.00	151.25
	3184	CG	PRO	B	533	84.400	124.997	163.830	1.00	156.89
	3185	C	PRO	B	533	81.477	125.558	163.605	1.00	132.46
	3186	O	PRO	B	533	80.902	126.440	162.963	1.00	100.35
55	3187	N	SER	B	534	81.320	124.256	163.383	1.00	143.66

	3188	CA	SER	B	534	80.452	123.734	162.335	1.00	132.97
	3189	CB	SER	B	534	81.191	122.649	161.552	1.00	161.58
	3190	OG	SER	B	534	81.699	121.659	162.433	1.00	165.58
	3191	C	SER	B	534	79.150	123.167	162.880	1.00	119.62
	3192	O	SER	B	534	78.478	122.386	162.208	1.00	111.21
	3193	N	GLN	B	535	78.797	123.562	164.097	1.00	121.56
	3194	CA	GLN	B	535	77.567	123.100	164.729	1.00	104.19
	3195	CB	GLN	B	535	76.364	123.514	163.874	1.00	39.24
	3196	CG	GLN	B	535	76.251	125.023	163.741	1.00	73.06
	3197	CD	GLN	B	535	76.192	125.485	162.297	1.00	105.92
	3198	OE1	GLN	B	535	76.935	124.993	161.445	1.00	122.35
	3199	NE2	GLN	B	535	75.317	126.449	162.017	1.00	116.95
	3200	C	GLN	B	535	77.588	121.590	164.945	1.00	81.66
	3201	O	GLN	B	535	76.565	120.977	165.244	1.00	75.14
	3202	N	THR	B	536	78.772	121.005	164.809	1.00	75.59
	3203	CA	THR	B	536	78.960	119.571	164.983	1.00	73.02
	3204	CB	THR	B	536	79.677	118.967	163.771	1.00	96.53
	3205	OG1	THR	B	536	78.861	119.117	162.604	1.00	138.70
	3206	CG2	THR	B	536	79.973	117.509	164.005	1.00	87.18
	3207	C	THR	B	536	79.825	119.321	166.200	1.00	72.59
	3208	O	THR	B	536	80.514	120.215	166.672	1.00	108.65
	3209	N	VAL	B	537	79.798	118.095	166.694	1.00	58.96
	3210	CA	VAL	B	537	80.600	117.708	167.847	1.00	83.66
	3211	CB	VAL	B	537	79.969	118.190	169.146	1.00	52.09
	3212	CG1	VAL	B	537	80.474	117.351	170.311	1.00	68.77
	3213	CG2	VAL	B	537	80.317	119.645	169.366	1.00	119.61
	3214	C	VAL	B	537	80.723	116.195	167.904	1.00	99.63
	3215	O	VAL	B	537	79.719	115.495	167.960	1.00	109.69
	3216	N	GLN	B	538	81.947	115.685	167.904	1.00	100.40
	3217	CA	GLN	B	538	82.128	114.242	167.931	1.00	90.82
	3218	CB	GLN	B	538	82.389	113.741	166.508	1.00	92.68
	3219	CG	GLN	B	538	83.519	114.462	165.790	1.00	69.71
	3220	CD	GLN	B	538	83.524	114.199	164.292	1.00	97.76
	3221	OE1	GLN	B	538	82.734	114.776	163.543	1.00	78.04
	3222	NE2	GLN	B	538	84.410	113.314	163.850	1.00	116.83
	3223	C	GLN	B	538	83.238	113.781	168.859	1.00	75.38
	3224	O	GLN	B	538	84.090	114.568	169.262	1.00	96.22
	3225	N	ARG	B	539	83.206	112.500	169.206	1.00	51.75
	3226	CA	ARG	B	539	84.215	111.907	170.074	1.00	99.09
	3227	CB	ARG	B	539	83.719	111.803	171.517	1.00	100.20
	3228	CG	ARG	B	539	84.820	111.481	172.533	1.00	145.36
	3229	CD	ARG	B	539	85.250	112.726	173.313	1.00	159.80
	3230	NE	ARG	B	539	85.363	113.903	172.451	1.00	167.91
	3231	CZ	ARG	B	539	85.663	115.127	172.880	1.00	150.28
	3232	NH1	ARG	B	539	85.887	115.344	174.170	1.00	164.72
	3233	NH2	ARG	B	539	85.726	116.136	172.017	1.00	114.07
	3234	C	ARG	B	539	84.493	110.512	169.547	1.00	119.86
	3235	O	ARG	B	539	83.580	109.700	169.426	1.00	90.13
	3236	N	ALA	B	540	85.753	110.236	169.234	1.00	128.12
	3237	CA	ALA	B	540	86.136	108.933	168.712	1.00	89.16
	3238	CB	ALA	B	540	87.531	109.015	168.111	1.00	124.98
	3239	C	ALA	B	540	86.100	107.866	169.796	1.00	76.22
	3240	O	ALA	B	540	86.009	108.171	170.980	1.00	109.84
	3241	N	VAL	B	541	86.173	106.612	169.376	1.00	60.52
	3242	CA	VAL	B	541	86.179	105.491	170.303	1.00	86.69

	3243	CB	VAL	B	541	84.770	105.139	170.724	1.00	87.58
	3244	CG1	VAL	B	541	84.005	104.682	169.512	1.00	77.89
	3245	CG2	VAL	B	541	84.785	104.059	171.807	1.00	52.44
	3246	C	VAL	B	541	86.786	104.283	169.597	1.00	102.20
5	3247	O	VAL	B	541	87.163	104.375	168.430	1.00	152.01
	3248	N	SER	B	542	86.882	103.159	170.306	1.00	105.84
	3249	CA	SER	B	542	87.426	101.922	169.748	1.00	89.13
	3250	CB	SER	B	542	88.722	102.199	168.975	1.00	113.60
	3251	OG	SER	B	542	89.682	102.852	169.791	1.00	119.14
10	3252	C	SER	B	542	87.713	100.893	170.829	1.00	69.68
	3253	O	SER	B	542	87.935	101.248	171.987	1.00	134.26
	3254	N	VAL	B	543	87.710	99.618	170.452	1.00	64.03
	3255	CA	VAL	B	543	88.017	98.550	171.401	1.00	113.44
	3256	CB	VAL	B	543	87.339	97.221	171.023	1.00	126.85
15	3257	CG1	VAL	B	543	87.101	96.404	172.285	1.00	62.70
	3258	CG2	VAL	B	543	86.055	97.470	170.223	1.00	22.03
	3259	C	VAL	B	543	89.530	98.308	171.372	1.00	152.87
	3260	O	VAL	B	543	90.183	98.571	170.361	1.00	170.87
	3261	N	ASN	B	544	90.079	97.799	172.472	1.00	147.76
20	3262	CA	ASN	B	544	91.511	97.522	172.561	1.00	158.75
	3263	CB	ASN	B	544	91.944	96.576	171.431	1.00	162.14
	3264	CG	ASN	B	544	91.163	95.267	171.423	1.00	149.81
	3265	OD1	ASN	B	544	91.128	94.541	172.417	1.00	152.63
	3266	ND2	ASN	B	544	90.540	94.958	170.289	1.00	96.95
25	3267	C	ASN	B	544	92.336	98.814	172.498	1.00	165.23
	3268	O	ASN	B	544	93.135	99.041	173.435	1.00	169.09
	3269	OXT	ASN	B	544	92.179	99.582	171.517	1.00	91.11
	3270	C1	NAG	B	694	43.351	106.499	163.692	1.00	45.89
	3271	C2	NAG	B	694	43.324	107.210	165.050	1.00	60.23
30	3272	N2	NAG	B	694	42.009	107.764	165.311	1.00	56.36
	3273	C7	NAG	B	694	41.107	107.072	166.005	1.00	75.39
	3274	O7	NAG	B	694	41.224	105.878	166.283	1.00	71.41
	3275	C8	NAG	B	694	39.876	107.819	166.449	1.00	22.03
	3276	C3	NAG	B	694	44.367	108.326	165.119	1.00	58.80
35	3277	O3	NAG	B	694	44.468	108.774	166.459	1.00	74.72
	3278	C4	NAG	B	694	45.745	107.860	164.653	1.00	56.10
	3279	O4	NAG	B	694	46.595	109.009	164.472	1.00	83.05
	3280	C5	NAG	B	694	45.633	107.121	163.324	1.00	25.95
	3281	O5	NAG	B	694	44.683	106.052	163.418	1.00	53.24
40	3282	C6	NAG	B	694	46.944	106.492	162.896	1.00	119.03
	3283	O6	NAG	B	694	46.718	105.307	162.144	1.00	138.62
	3284	C1	NAG	B	695	47.667	109.149	165.334	1.00	105.64
	3285	C2	NAG	B	695	48.912	109.587	164.537	1.00	59.77
	3286	N2	NAG	B	695	49.357	108.488	163.700	1.00	93.15
45	3287	C7	NAG	B	695	49.909	108.731	162.516	1.00	103.18
	3288	O7	NAG	B	695	51.131	108.754	162.340	1.00	136.64
	3289	C8	NAG	B	695	48.960	108.985	161.349	1.00	60.78
	3290	C3	NAG	B	695	50.062	110.046	165.456	1.00	79.33
	3291	O3	NAG	B	695	51.051	110.680	164.656	1.00	98.62
50	3292	C4	NAG	B	695	49.530	111.028	166.523	1.00	100.15
	3293	O4	NAG	B	695	50.546	111.348	167.496	1.00	82.39
	3294	C5	NAG	B	695	48.357	110.377	167.236	1.00	125.01
	3295	O5	NAG	B	695	47.306	110.143	166.294	1.00	76.78
	3296	C6	NAG	B	695	47.797	111.249	168.331	1.00	149.78
55	3297	O6	NAG	B	695	46.422	110.979	168.540	1.00	106.46

	3298	C1	MAN	B	696	51.371	112.429	167.246	1.00	73.26
	3299	C2	MAN	B	696	51.896	112.953	168.555	1.00	85.84
	3300	O2	MAN	B	696	52.572	111.906	169.203	1.00	84.25
	3301	C3	MAN	B	696	52.858	114.113	168.311	1.00	120.67
5	3302	O3	MAN	B	696	53.494	114.526	169.543	1.00	161.15
	3303	C4	MAN	B	696	53.939	113.688	167.318	1.00	142.38
	3304	O4	MAN	B	696	54.644	114.828	166.907	1.00	158.25
	3305	C5	MAN	B	696	53.376	112.998	166.077	1.00	122.76
	3306	O5	MAN	B	696	52.478	111.940	166.480	1.00	129.27
10	3307	C6	MAN	B	696	54.495	112.437	165.214	1.00	121.56
	3308	O6	MAN	B	696	54.271	111.063	164.855	1.00	154.87
	3309	C1	MAN	B	697	55.439	110.276	165.023	1.00	145.40
	3310	C2	MAN	B	697	56.117	110.375	166.417	1.00	145.77
	3311	O2	MAN	B	697	57.047	109.270	166.517	1.00	146.40
15	3312	C3	MAN	B	697	56.937	111.658	166.557	1.00	141.88
	3313	O3	MAN	B	697	57.844	111.476	167.629	1.00	137.62
	3314	C4	MAN	B	697	57.782	111.951	165.323	1.00	141.83
	3315	O4	MAN	B	697	58.361	113.247	165.387	1.00	139.00
	3316	C5	MAN	B	697	57.018	111.797	164.042	1.00	143.82
20	3317	O5	MAN	B	697	56.422	110.499	164.016	1.00	146.27
	3318	C6	MAN	B	697	57.919	111.862	162.860	1.00	148.17
	3319	O6	MAN	B	697	57.262	111.446	161.673	1.00	150.80
	3320	C1	MAN	B	698	52.693	115.215	170.457	1.00	166.73
	3321	C2	MAN	B	698	53.464	116.407	171.056	1.00	180.10
25	3322	O2	MAN	B	698	52.557	117.261	171.748	1.00	145.07
	3323	C3	MAN	B	698	54.563	115.916	172.016	1.00	172.30
	3324	O3	MAN	B	698	55.188	117.024	172.657	1.00	137.27
	3325	C4	MAN	B	698	53.964	114.962	173.060	1.00	164.34
	3326	O4	MAN	B	698	54.992	114.436	173.885	1.00	140.37
30	3327	C5	MAN	B	698	53.231	113.819	172.351	1.00	150.05
	3328	O5	MAN	B	698	52.208	114.363	171.491	1.00	142.54
	3329	C6	MAN	B	698	52.553	112.858	173.311	1.00	146.09
	3330	O6	MAN	B	698	51.158	112.769	173.056	1.00	158.71
	3331	C1	MAN	B	699	56.966	108.431	167.643	1.00	147.68
35	3332	C2	MAN	B	699	58.038	108.848	168.676	1.00	149.11
	3333	O2	MAN	B	699	57.797	108.220	169.928	1.00	144.31
	3334	C3	MAN	B	699	59.464	108.512	168.172	1.00	149.80
	3335	O3	MAN	B	699	60.421	108.765	169.197	1.00	142.63
	3336	C4	MAN	B	699	59.578	107.043	167.743	1.00	151.96
40	3337	O4	MAN	B	699	60.851	106.815	167.127	1.00	149.52
	3338	C5	MAN	B	699	58.427	106.645	166.780	1.00	152.87
	3339	O5	MAN	B	699	57.110	107.042	167.306	1.00	150.31
	3340	C6	MAN	B	699	58.378	105.138	166.486	1.00	152.00
	3341	O6	MAN	B	699	58.826	104.348	167.584	1.00	155.30
45	3342	C	CYS	D	329	40.977	121.748	178.634	1.00	210.29
	3343	O	CYS	D	329	41.782	122.273	179.404	1.00	189.25
	3344	CB	CYS	D	329	41.494	121.206	176.231	1.00	224.93
	3345	SG	CYS	D	329	39.884	121.730	175.555	1.00	250.42
	3346	N	CYS	D	329	40.558	119.454	177.703	1.00	206.24
50	3347	CA	CYS	D	329	41.438	120.654	177.662	1.00	208.57
	3348	N	ASP	D	330	39.687	122.084	178.603	1.00	212.05
	3349	CA	ASP	D	330	39.131	123.119	179.482	1.00	192.97
	3350	CB	ASP	D	330	38.840	124.395	178.679	1.00	200.39
	3351	CG	ASP	D	330	38.321	125.535	179.549	1.00	207.96
55	3352	OD1	ASP	D	330	37.203	125.420	180.100	1.00	182.28

	3353	OD2	ASP	D	330	39.037	126.552	179.681	1.00	213.37
	3354	C	ASP	D	330	37.854	122.657	180.187	1.00	188.18
	3355	O	ASP	D	330	37.908	122.095	181.282	1.00	170.40
	3356	N	SER	D	331	36.707	122.905	179.557	1.00	186.14
5	3357	CA	SER	D	331	35.419	122.512	180.123	1.00	155.83
	3358	CB	SER	D	331	34.266	123.184	179.364	1.00	152.11
	3359	OG	SER	D	331	34.055	122.582	178.092	1.00	95.70
	3360	C	SER	D	331	35.242	120.995	180.068	1.00	163.80
	3361	O	SER	D	331	34.998	120.366	181.098	1.00	161.57
10	3362	N	ASN	D	332	35.368	120.419	178.869	1.00	159.48
	3363	CA	ASN	D	332	35.214	118.978	178.678	1.00	122.47
	3364	CB	ASN	D	332	35.786	118.530	177.325	1.00	172.30
	3365	CG	ASN	D	332	37.269	118.836	177.170	1.00	223.31
	3366	OD1	ASN	D	332	37.916	119.341	178.087	1.00	239.48
15	3367	ND2	ASN	D	332	37.816	118.520	175.998	1.00	237.24
	3368	C	ASN	D	332	35.874	118.205	179.816	1.00	105.80
	3369	O	ASN	D	332	37.091	118.207	179.975	1.00	93.15
	3370	N	PRO	D	333	35.064	117.539	180.644	1.00	64.26
	3371	CD	PRO	D	333	33.600	117.604	180.724	1.00	41.20
20	3372	CA	PRO	D	333	35.595	116.778	181.771	1.00	41.52
	3373	CB	PRO	D	333	34.363	116.548	182.633	1.00	35.93
	3374	CG	PRO	D	333	33.402	117.622	182.204	1.00	77.83
	3375	C	PRO	D	333	36.222	115.480	181.314	1.00	54.76
	3376	O	PRO	D	333	35.858	114.951	180.272	1.00	34.59
25	3377	N	ARG	D	334	37.160	114.976	182.107	1.00	19.96
	3378	CA	ARG	D	334	37.866	113.731	181.813	1.00	40.10
	3379	CB	ARG	D	334	39.389	113.936	181.935	1.00	60.92
	3380	CG	ARG	D	334	40.245	112.697	181.633	1.00	28.56
	3381	CD	ARG	D	334	41.745	112.986	181.457	1.00	78.41
30	3382	NE	ARG	D	334	42.377	112.028	180.545	1.00	73.15
	3383	CZ	ARG	D	334	42.757	112.326	179.306	1.00	100.07
	3384	NH1	ARG	D	334	42.575	113.553	178.841	1.00	59.54
	3385	NH2	ARG	D	334	43.299	111.401	178.525	1.00	145.40
	3386	C	ARG	D	334	37.378	112.727	182.841	1.00	5.42
35	3387	O	ARG	D	334	37.095	113.087	183.979	1.00	48.58
	3388	N	GLY	D	335	37.273	111.473	182.444	1.00	20.86
	3389	CA	GLY	D	335	36.759	110.464	183.343	1.00	41.07
	3390	C	GLY	D	335	37.790	109.753	184.165	1.00	29.22
	3391	O	GLY	D	335	38.979	109.833	183.880	1.00	46.30
40	3392	N	VAL	D	336	37.326	109.034	185.179	1.00	37.28
	3393	CA	VAL	D	336	38.220	108.307	186.063	1.00	5.96
	3394	CB	VAL	D	336	37.470	107.553	187.153	1.00	31.42
	3395	CG1	VAL	D	336	38.326	106.455	187.693	1.00	28.30
	3396	CG2	VAL	D	336	37.136	108.471	188.264	1.00	26.00
45	3397	C	VAL	D	336	39.053	107.302	185.328	1.00	38.88
	3398	O	VAL	D	336	38.554	106.584	184.463	1.00	39.16
	3399	N	SER	D	337	40.325	107.252	185.712	1.00	43.15
	3400	CA	SER	D	337	41.306	106.342	185.141	1.00	54.37
	3401	CB	SER	D	337	42.393	107.149	184.445	1.00	48.14
50	3402	OG	SER	D	337	41.836	108.240	183.724	1.00	87.47
	3403	C	SER	D	337	41.904	105.601	186.321	1.00	32.96
	3404	O	SER	D	337	41.957	106.143	187.413	1.00	38.71
	3405	N	ALA	D	338	42.330	104.361	186.128	1.00	43.73
	3406	CA	ALA	D	338	42.942	103.622	187.234	1.00	32.03
55	3407	CB	ALA	D	338	42.005	102.619	187.813	1.00	13.06

	3408	C	ALA	D	338	44.176	102.928	186.739	1.00	38.96
	3409	O	ALA	D	338	44.243	102.514	185.591	1.00	58.49
	3410	N	TYR	D	339	45.148	102.798	187.626	1.00	53.04
	3411	CA	TYR	D	339	46.417	102.195	187.298	1.00	41.03
	3412	CB	TYR	D	339	47.422	103.306	187.101	1.00	30.65
	3413	CG	TYR	D	339	46.976	104.376	186.120	1.00	5.42
	3414	CD1	TYR	D	339	46.755	105.677	186.536	1.00	64.60
	3415	CE1	TYR	D	339	46.456	106.687	185.625	1.00	68.13
	3416	CD2	TYR	D	339	46.873	104.104	184.765	1.00	66.56
	3417	CE2	TYR	D	339	46.575	105.104	183.851	1.00	42.43
	3418	CZ	TYR	D	339	46.373	106.396	184.287	1.00	52.17
	3419	OH	TYR	D	339	46.134	107.408	183.379	1.00	96.24
	3420	C	TYR	D	339	46.835	101.285	188.439	1.00	48.87
	3421	O	TYR	D	339	46.362	101.445	189.558	1.00	76.65
	3422	N	LEU	D	340	47.730	100.345	188.175	1.00	64.84
	3423	CA	LEU	D	340	48.140	99.410	189.213	1.00	61.58
	3424	CB	LEU	D	340	47.263	98.177	189.122	1.00	18.16
	3425	CG	LEU	D	340	47.443	97.047	190.119	1.00	25.80
	3426	CD1	LEU	D	340	47.122	97.518	191.509	1.00	65.83
	3427	CD2	LEU	D	340	46.525	95.915	189.742	1.00	77.47
	3428	C	LEU	D	340	49.597	99.023	189.051	1.00	81.86
	3429	O	LEU	D	340	49.935	98.238	188.174	1.00	80.36
	3430	N	SER	D	341	50.456	99.560	189.912	1.00	80.46
	3431	CA	SER	D	341	51.886	99.302	189.822	1.00	85.77
	3432	CB	SER	D	341	52.656	100.405	190.549	1.00	101.32
	3433	OG	SER	D	341	54.041	100.346	190.248	1.00	155.34
	3434	C	SER	D	341	52.304	97.947	190.358	1.00	81.11
	3435	O	SER	D	341	51.698	97.429	191.277	1.00	77.74
	3436	N	ARG	D	342	53.355	97.388	189.766	1.00	106.18
	3437	CA	ARG	D	342	53.912	96.091	190.150	1.00	44.48
	3438	CB	ARG	D	342	54.380	95.361	188.892	1.00	103.52
	3439	CG	ARG	D	342	55.115	96.289	187.906	1.00	146.45
	3440	CD	ARG	D	342	55.845	95.557	186.765	1.00	148.55
	3441	NE	ARG	D	342	54.964	95.031	185.722	1.00	106.07
	3442	CZ	ARG	D	342	54.265	93.904	185.823	1.00	125.40
	3443	NH1	ARG	D	342	54.337	93.159	186.925	1.00	81.34
	3444	NH2	ARG	D	342	53.479	93.525	184.823	1.00	138.83
	3445	C	ARG	D	342	55.100	96.277	191.117	1.00	93.34
	3446	O	ARG	D	342	55.835	97.267	191.044	1.00	84.98
	3447	N	PRO	D	343	55.309	95.312	192.025	1.00	51.92
	3448	CD	PRO	D	343	54.613	94.020	192.055	1.00	46.08
	3449	CA	PRO	D	343	56.390	95.336	193.017	1.00	37.46
	3450	CB	PRO	D	343	56.323	93.946	193.638	1.00	54.05
	3451	CG	PRO	D	343	54.925	93.534	193.435	1.00	34.48
	3452	C	PRO	D	343	57.728	95.556	192.357	1.00	31.46
	3453	O	PRO	D	343	58.023	94.920	191.352	1.00	83.41
	3454	N	SER	D	344	58.555	96.430	192.906	1.00	68.87
	3455	CA	SER	D	344	59.859	96.648	192.298	1.00	74.31
	3456	CB	SER	D	344	60.476	97.969	192.781	1.00	78.99
	3457	OG	SER	D	344	60.734	97.939	194.173	1.00	86.16
	3458	C	SER	D	344	60.764	95.480	192.681	1.00	78.78
	3459	O	SER	D	344	60.571	94.858	193.730	1.00	64.79
	3460	N	PRO	D	345	61.744	95.149	191.822	1.00	78.82
	3461	CD	PRO	D	345	62.114	95.844	190.579	1.00	86.56
	3462	CA	PRO	D	345	62.673	94.054	192.096	1.00	69.52

	3463	CB	PRO	D	345	63.792	94.311	191.101	1.00	81.00
	3464	CG	PRO	D	345	63.078	94.883	189.947	1.00	56.65
	3465	C	PRO	D	345	63.162	94.234	193.523	1.00	87.38
	3466	O	PRO	D	345	63.009	93.356	194.382	1.00	70.47
5	3467	N	PHE	D	346	63.745	95.408	193.750	1.00	57.09
	3468	CA	PHE	D	346	64.270	95.788	195.044	1.00	47.21
	3469	CB	PHE	D	346	64.603	97.279	195.036	1.00	62.17
	3470	CG	PHE	D	346	65.157	97.779	196.334	1.00	92.21
	3471	CD1	PHE	D	346	66.368	97.309	196.814	1.00	77.54
10	3472	CD2	PHE	D	346	64.459	98.712	197.085	1.00	130.01
	3473	CE1	PHE	D	346	66.874	97.759	198.016	1.00	101.47
	3474	CE2	PHE	D	346	64.958	99.170	198.294	1.00	121.98
	3475	CZ	PHE	D	346	66.167	98.693	198.761	1.00	136.63
	3476	C	PHE	D	346	63.300	95.463	196.180	1.00	61.69
15	3477	O	PHE	D	346	63.557	94.562	196.976	1.00	58.05
	3478	N	ASP	D	347	62.186	96.182	196.250	1.00	49.53
	3479	CA	ASP	D	347	61.199	95.958	197.302	1.00	60.77
	3480	CB	ASP	D	347	59.939	96.792	197.044	1.00	97.33
	3481	CG	ASP	D	347	60.121	98.260	197.380	1.00	120.23
20	3482	OD1	ASP	D	347	60.197	98.590	198.583	1.00	142.30
	3483	OD2	ASP	D	347	60.189	99.084	196.443	1.00	147.88
	3484	C	ASP	D	347	60.791	94.494	197.407	1.00	79.99
	3485	O	ASP	D	347	60.144	94.086	198.373	1.00	51.27
	3486	N	LEU	D	348	61.191	93.697	196.427	1.00	54.00
25	3487	CA	LEU	D	348	60.791	92.304	196.400	1.00	73.58
	3488	CB	LEU	D	348	60.293	91.977	194.991	1.00	43.65
	3489	CG	LEU	D	348	59.764	90.586	194.663	1.00	61.62
	3490	CD1	LEU	D	348	58.851	90.063	195.737	1.00	73.74
	3491	CD2	LEU	D	348	59.041	90.673	193.342	1.00	84.11
30	3492	C	LEU	D	348	61.823	91.287	196.838	1.00	79.18
	3493	O	LEU	D	348	61.456	90.240	197.381	1.00	67.98
	3494	N	PHE	D	349	63.103	91.596	196.617	1.00	89.01
	3495	CA	PHE	D	349	64.195	90.681	196.959	1.00	97.99
	3496	CB	PHE	D	349	64.993	90.401	195.706	1.00	91.42
35	3497	CG	PHE	D	349	64.191	89.710	194.656	1.00	89.32
	3498	CD1	PHE	D	349	64.403	89.967	193.315	1.00	93.99
	3499	CD2	PHE	D	349	63.194	88.804	195.021	1.00	58.86
	3500	CE1	PHE	D	349	63.633	89.339	192.352	1.00	60.78
	3501	CE2	PHE	D	349	62.420	88.171	194.061	1.00	91.28
40	3502	CZ	PHE	D	349	62.639	88.439	192.724	1.00	94.91
	3503	C	PHE	D	349	65.098	91.150	198.076	1.00	102.56
	3504	O	PHE	D	349	65.470	90.369	198.955	1.00	116.27
	3505	N	ILE	D	350	65.464	92.422	198.033	1.00	96.29
	3506	CA	ILE	D	350	66.276	92.993	199.088	1.00	73.68
45	3507	CB	ILE	D	350	66.804	94.381	198.700	1.00	73.26
	3508	CG2	ILE	D	350	67.594	94.970	199.850	1.00	90.70
	3509	CG1	ILE	D	350	67.638	94.282	197.428	1.00	62.89
	3510	CD1	ILE	D	350	68.682	93.207	197.474	1.00	77.68
	3511	C	ILE	D	350	65.337	93.162	200.286	1.00	91.79
50	3512	O	ILE	D	350	65.229	92.277	201.143	1.00	96.73
	3513	N	ARG	D	351	64.639	94.299	200.302	1.00	79.05
	3514	CA	ARG	D	351	63.696	94.661	201.356	1.00	77.91
	3515	CB	ARG	D	351	62.908	95.894	200.909	1.00	81.92
	3516	CG	ARG	D	351	62.429	96.796	202.033	1.00	114.59
55	3517	CD	ARG	D	351	62.218	98.216	201.513	1.00	129.04

	3518	NE	ARG	D	351	61.772	99.135	202.556	1.00	176.58
	3519	CZ	ARG	D	351	60.594	99.057	203.165	1.00	194.68
	3520	NH1	ARG	D	351	59.738	98.100	202.835	1.00	199.64
	3521	NH2	ARG	D	351	60.271	99.937	204.105	1.00	191.83
	3522	C	ARG	D	351	62.738	93.529	201.737	1.00	87.28
	3523	O	ARG	D	351	62.129	93.558	202.807	1.00	85.89
	3524	N	LYS	D	352	62.620	92.536	200.860	1.00	64.64
	3525	CA	LYS	D	352	61.754	91.375	201.066	1.00	110.09
	3526	CB	LYS	D	352	62.443	90.351	201.977	1.00	137.68
	3527	CG	LYS	D	352	63.695	89.710	201.380	1.00	164.74
	3528	CD	LYS	D	352	64.045	88.410	202.099	1.00	184.77
	3529	CE	LYS	D	352	65.381	87.834	201.642	1.00	171.68
	3530	NZ	LYS	D	352	66.539	88.623	202.153	1.00	185.42
	3531	C	LYS	D	352	60.339	91.659	201.587	1.00	121.79
	3532	O	LYS	D	352	59.714	90.793	202.198	1.00	115.18
	3533	N	SER	D	353	59.841	92.869	201.344	1.00	129.12
	3534	CA	SER	D	353	58.484	93.265	201.740	1.00	107.18
	3535	CB	SER	D	353	58.506	94.174	202.975	1.00	122.87
	3536	OG	SER	D	353	59.158	95.404	202.707	1.00	166.93
	3537	C	SER	D	353	57.907	94.012	200.534	1.00	102.01
	3538	O	SER	D	353	57.957	95.243	200.446	1.00	86.01
	3539	N	PRO	D	354	57.350	93.261	199.578	1.00	86.76
	3540	CD	PRO	D	354	57.251	91.797	199.555	1.00	96.08
	3541	CA	PRO	D	354	56.770	93.816	198.361	1.00	78.36
	3542	CB	PRO	D	354	56.785	92.630	197.393	1.00	84.14
	3543	CG	PRO	D	354	57.526	91.526	198.127	1.00	77.25
	3544	C	PRO	D	354	55.367	94.332	198.547	1.00	94.58
	3545	O	PRO	D	354	54.605	93.797	199.350	1.00	69.20
	3546	N	THR	D	355	55.033	95.366	197.781	1.00	81.15
	3547	CA	THR	D	355	53.706	95.957	197.813	1.00	52.66
	3548	CB	THR	D	355	53.598	97.082	198.827	1.00	55.40
	3549	OG1	THR	D	355	54.557	98.101	198.513	1.00	77.41
	3550	CG2	THR	D	355	53.816	96.551	200.232	1.00	118.83
	3551	C	THR	D	355	53.328	96.554	196.475	1.00	73.36
	3552	O	THR	D	355	54.123	97.269	195.852	1.00	60.58
	3553	N	ILE	D	356	52.100	96.261	196.054	1.00	68.63
	3554	CA	ILE	D	356	51.550	96.771	194.809	1.00	71.72
	3555	CB	ILE	D	356	50.725	95.712	194.105	1.00	33.12
	3556	CG2	ILE	D	356	51.621	94.618	193.613	1.00	84.96
	3557	CG1	ILE	D	356	49.693	95.138	195.059	1.00	69.76
	3558	CD1	ILE	D	356	48.895	93.992	194.466	1.00	78.12
	3559	C	ILE	D	356	50.660	97.956	195.140	1.00	56.65
	3560	O	ILE	D	356	50.092	98.020	196.214	1.00	40.32
	3561	N	THR	D	357	50.527	98.886	194.210	1.00	41.53
	3562	CA	THR	D	357	49.738	100.075	194.453	1.00	56.47
	3563	CB	THR	D	357	50.661	101.268	194.609	1.00	44.57
	3564	OG1	THR	D	357	51.732	100.908	195.484	1.00	86.28
	3565	CG2	THR	D	357	49.919	102.440	195.180	1.00	70.27
	3566	C	THR	D	357	48.719	100.390	193.367	1.00	61.21
	3567	O	THR	D	357	49.043	100.408	192.182	1.00	65.37
	3568	N	CYS	D	358	47.487	100.656	193.794	1.00	57.66
	3569	CA	CYS	D	358	46.388	100.989	192.898	1.00	62.45
	3570	C	CYS	D	358	46.155	102.478	192.983	1.00	45.63
	3571	O	CYS	D	358	45.867	102.993	194.054	1.00	74.78
	3572	CB	CYS	D	358	45.135	100.263	193.341	1.00	61.30

	3573	SG	CYS	D	358	43.775	100.299	192.140	1.00	68.08
	3574	N	LEU	D	359	46.272	103.174	191.864	1.00	41.70
	3575	CA	LEU	D	359	46.105	104.616	191.868	1.00	25.08
	3576	CB	LEU	D	359	47.404	105.279	191.410	1.00	65.10
	3577	CG	LEU	D	359	47.322	106.716	190.905	1.00	16.89
	3578	CD1	LEU	D	359	46.716	107.566	191.963	1.00	57.67
	3579	CD2	LEU	D	359	48.703	107.229	190.549	1.00	96.64
	3580	C	LEU	D	359	44.954	105.063	190.986	1.00	44.20
	3581	O	LEU	D	359	44.956	104.830	189.784	1.00	68.36
	3582	N	VAL	D	360	43.971	105.715	191.591	1.00	50.01
	3583	CA	VAL	D	360	42.821	106.193	190.853	1.00	29.75
	3584	CB	VAL	D	360	41.539	105.909	191.602	1.00	34.70
	3585	CG1	VAL	D	360	40.388	106.459	190.821	1.00	38.83
	3586	CG2	VAL	D	360	41.365	104.422	191.810	1.00	28.01
	3587	C	VAL	D	360	42.927	107.681	190.661	1.00	28.40
	3588	O	VAL	D	360	43.209	108.404	191.601	1.00	60.69
	3589	N	VAL	D	361	42.677	108.146	189.450	1.00	28.27
	3590	CA	VAL	D	361	42.771	109.574	189.156	1.00	32.16
	3591	CB	VAL	D	361	44.007	109.853	188.272	1.00	10.08
	3592	CG1	VAL	D	361	44.974	108.690	188.387	1.00	49.51
	3593	CG2	VAL	D	361	43.595	110.013	186.820	1.00	48.77
	3594	C	VAL	D	361	41.525	110.131	188.458	1.00	26.83
	3595	O	VAL	D	361	40.695	109.389	187.937	1.00	48.72
	3596	N	ASP	D	362	41.422	111.452	188.433	1.00	44.02
	3597	CA	ASP	D	362	40.308	112.142	187.804	1.00	31.26
	3598	CB	ASP	D	362	40.227	111.794	186.324	1.00	57.54
	3599	CG	ASP	D	362	41.377	112.380	185.527	1.00	99.45
	3600	OD1	ASP	D	362	41.751	113.542	185.804	1.00	59.82
	3601	OD2	ASP	D	362	41.893	111.684	184.620	1.00	97.18
	3602	C	ASP	D	362	38.945	111.946	188.458	1.00	45.28
	3603	O	ASP	D	362	37.914	112.146	187.816	1.00	58.17
	3604	N	LEU	D	363	38.943	111.554	189.730	1.00	31.65
	3605	CA	LEU	D	363	37.709	111.405	190.496	1.00	30.37
	3606	CB	LEU	D	363	37.964	110.712	191.820	1.00	14.90
	3607	CG	LEU	D	363	38.139	109.208	191.819	1.00	39.19
	3608	CD1	LEU	D	363	38.611	108.750	193.177	1.00	47.04
	3609	CD2	LEU	D	363	36.839	108.553	191.480	1.00	35.75
	3610	C	LEU	D	363	37.243	112.814	190.820	1.00	68.38
	3611	O	LEU	D	363	38.045	113.751	190.805	1.00	53.90
	3612	N	ALA	D	364	35.962	112.974	191.142	1.00	116.09
	3613	CA	ALA	D	364	35.443	114.297	191.475	1.00	94.58
	3614	CB	ALA	D	364	34.731	114.906	190.280	1.00	92.82
	3615	C	ALA	D	364	34.498	114.228	192.656	1.00	118.54
	3616	O	ALA	D	364	33.729	113.273	192.797	1.00	129.25
	3617	N	PRO	D	365	34.548	115.252	193.524	1.00	128.97
	3618	CD	PRO	D	365	35.391	116.455	193.354	1.00	57.81
	3619	CA	PRO	D	365	33.710	115.360	194.723	1.00	105.98
	3620	CB	PRO	D	365	33.666	116.860	194.958	1.00	121.84
	3621	CG	PRO	D	365	35.087	117.254	194.616	1.00	78.18
	3622	C	PRO	D	365	32.323	114.734	194.549	1.00	91.22
	3623	O	PRO	D	365	31.436	115.298	193.916	1.00	85.50
	3624	N	SER	D	366	32.162	113.542	195.107	1.00	132.49
	3625	CA	SER	D	366	30.904	112.816	195.033	1.00	136.44
	3626	CB	SER	D	366	31.149	111.400	194.503	1.00	121.82
	3627	OG	SER	D	366	32.105	110.710	195.302	1.00	115.17

	3628	C	SER	D	366	30.313	112.752	196.438	1.00	176.44
	3629	O	SER	D	366	31.031	112.918	197.428	1.00	164.25
	3630	N	LYS	D	367	29.007	112.523	196.524	1.00	189.75
	3631	CA	LYS	D	367	28.341	112.430	197.819	1.00	181.41
	3632	CB	LYS	D	367	26.896	112.910	197.720	1.00	196.81
	3633	CG	LYS	D	367	26.739	114.334	197.233	1.00	225.05
	3634	CD	LYS	D	367	27.059	115.373	198.291	1.00	212.98
	3635	CE	LYS	D	367	26.738	116.763	197.760	1.00	208.48
	3636	NZ	LYS	D	367	26.913	117.823	198.784	1.00	202.36
	3637	C	LYS	D	367	28.355	110.982	198.274	1.00	162.45
	3638	O	LYS	D	367	28.021	110.677	199.416	1.00	165.32
	3639	N	GLY	D	368	28.735	110.093	197.365	1.00	160.80
	3640	CA	GLY	D	368	28.791	108.685	197.696	1.00	152.04
	3641	C	GLY	D	368	30.217	108.220	197.912	1.00	174.77
	3642	O	GLY	D	368	31.174	108.928	197.582	1.00	170.78
	3643	N	THR	D	369	30.355	107.023	198.476	1.00	173.28
	3644	CA	THR	D	369	31.661	106.424	198.740	1.00	158.08
	3645	CB	THR	D	369	31.492	105.030	199.398	1.00	168.98
	3646	OG1	THR	D	369	30.447	105.089	200.378	1.00	140.65
	3647	CG2	THR	D	369	32.788	104.590	200.079	1.00	155.41
	3648	C	THR	D	369	32.375	106.253	197.396	1.00	126.97
	3649	O	THR	D	369	31.908	106.754	196.380	1.00	121.57
	3650	N	VAL	D	370	33.514	105.566	197.397	1.00	124.90
	3651	CA	VAL	D	370	34.254	105.306	196.166	1.00	58.92
	3652	CB	VAL	D	370	35.273	106.414	195.851	1.00	55.35
	3653	CG1	VAL	D	370	35.805	106.246	194.401	1.00	24.89
	3654	CG2	VAL	D	370	34.616	107.793	196.044	1.00	62.46
	3655	C	VAL	D	370	34.955	103.979	196.320	1.00	27.33
	3656	O	VAL	D	370	36.068	103.773	195.862	1.00	70.43
	3657	N	ASN	D	371	34.256	103.075	196.988	1.00	82.80
	3658	CA	ASN	D	371	34.734	101.724	197.243	1.00	69.31
	3659	CB	ASN	D	371	33.595	100.719	196.996	1.00	49.52
	3660	CG	ASN	D	371	32.950	100.229	198.274	1.00	104.67
	3661	OD1	ASN	D	371	32.407	101.025	199.043	1.00	117.80
	3662	ND2	ASN	D	371	32.979	98.919	198.497	1.00	168.88
	3663	C	ASN	D	371	35.958	101.252	196.469	1.00	80.11
	3664	O	ASN	D	371	35.988	101.271	195.234	1.00	50.10
	3665	N	LEU	D	372	36.972	100.847	197.218	1.00	87.75
	3666	CA	LEU	D	372	38.168	100.270	196.635	1.00	40.25
	3667	CB	LEU	D	372	39.399	101.036	197.078	1.00	51.63
	3668	CG	LEU	D	372	40.698	100.819	196.321	1.00	42.05
	3669	CD1	LEU	D	372	40.673	99.475	195.610	1.00	57.36
	3670	CD2	LEU	D	372	40.854	101.961	195.344	1.00	17.22
	3671	C	LEU	D	372	38.164	98.893	197.302	1.00	69.49
	3672	O	LEU	D	372	37.925	98.774	198.504	1.00	99.46
	3673	N	THR	D	373	38.398	97.852	196.524	1.00	50.31
	3674	CA	THR	D	373	38.367	96.516	197.078	1.00	38.63
	3675	CB	THR	D	373	36.958	95.894	196.859	1.00	63.65
	3676	OG1	THR	D	373	35.980	96.704	197.523	1.00	71.89
	3677	CG2	THR	D	373	36.905	94.478	197.408	1.00	89.69
	3678	C	THR	D	373	39.435	95.613	196.478	1.00	74.34
	3679	O	THR	D	373	39.493	95.440	195.262	1.00	67.92
	3680	N	TRP	D	374	40.273	95.032	197.335	1.00	71.85
	3681	CA	TRP	D	374	41.343	94.148	196.885	1.00	42.08
	3682	CB	TRP	D	374	42.566	94.309	197.769	1.00	57.45

	3683	CG	TRP	D	374	43.280	95.595	197.614	1.00	41.03
	3684	CD2	TRP	D	374	44.219	95.924	196.593	1.00	30.13
	3685	CE2	TRP	D	374	44.648	97.244	196.827	1.00	32.56
	3686	CE3	TRP	D	374	44.740	95.229	195.500	1.00	52.50
5	3687	CD1	TRP	D	374	43.176	96.697	198.410	1.00	58.12
	3688	NE1	TRP	D	374	44.000	97.697	197.944	1.00	31.82
	3689	CZ2	TRP	D	374	45.570	97.881	196.006	1.00	53.35
	3690	CZ3	TRP	D	374	45.658	95.864	194.684	1.00	47.95
	3691	CH2	TRP	D	374	46.064	97.175	194.939	1.00	23.35
10	3692	C	TRP	D	374	40.954	92.681	196.910	1.00	85.67
	3693	O	TRP	D	374	40.261	92.236	197.822	1.00	80.11
	3694	N	SER	D	375	41.434	91.916	195.936	1.00	64.91
	3695	CA	SER	D	375	41.110	90.496	195.878	1.00	80.39
	3696	CB	SER	D	375	39.737	90.325	195.236	1.00	121.93
15	3697	OG	SER	D	375	39.703	90.935	193.956	1.00	111.06
	3698	C	SER	D	375	42.135	89.659	195.114	1.00	105.31
	3699	O	SER	D	375	42.802	90.157	194.202	1.00	54.37
	3700	N	ARG	D	376	42.253	88.386	195.493	1.00	87.71
	3701	CA	ARG	D	376	43.174	87.466	194.831	1.00	90.92
20	3702	CB	ARG	D	376	43.974	86.665	195.854	1.00	101.35
	3703	CG	ARG	D	376	45.158	87.402	196.423	1.00	114.89
	3704	CD	ARG	D	376	46.249	86.437	196.863	1.00	123.05
	3705	NE	ARG	D	376	46.021	85.871	198.187	1.00	92.73
	3706	CZ	ARG	D	376	46.833	84.992	198.763	1.00	124.05
25	3707	NH1	ARG	D	376	47.920	84.580	198.128	1.00	110.55
	3708	NH2	ARG	D	376	46.567	84.534	199.978	1.00	162.37
	3709	C	ARG	D	376	42.420	86.499	193.927	1.00	117.75
	3710	O	ARG	D	376	41.260	86.168	194.186	1.00	105.90
	3711	N	ALA	D	377	43.082	86.039	192.871	1.00	99.06
30	3712	CA	ALA	D	377	42.453	85.109	191.944	1.00	110.56
	3713	CB	ALA	D	377	43.235	85.059	190.659	1.00	96.70
	3714	C	ALA	D	377	42.355	83.715	192.550	1.00	113.96
	3715	O	ALA	D	377	41.454	82.940	192.218	1.00	121.96
	3716	N	SER	D	378	43.288	83.400	193.441	1.00	100.05
35	3717	CA	SER	D	378	43.299	82.102	194.096	1.00	74.96
	3718	CB	SER	D	378	44.607	81.910	194.863	1.00	108.91
	3719	OG	SER	D	378	44.639	82.730	196.015	1.00	102.13
	3720	C	SER	D	378	42.119	81.973	195.060	1.00	87.98
	3721	O	SER	D	378	41.716	80.868	195.415	1.00	117.47
40	3722	N	GLY	D	379	41.569	83.105	195.478	1.00	88.22
	3723	CA	GLY	D	379	40.452	83.080	196.403	1.00	101.70
	3724	C	GLY	D	379	40.922	83.261	197.835	1.00	122.17
	3725	O	GLY	D	379	40.135	83.578	198.733	1.00	104.23
	3726	N	LYS	D	380	42.218	83.064	198.047	1.00	123.72
45	3727	CA	LYS	D	380	42.805	83.202	199.373	1.00	148.58
	3728	CB	LYS	D	380	44.260	82.727	199.348	1.00	164.15
	3729	CG	LYS	D	380	44.446	81.293	198.871	1.00	172.83
	3730	CD	LYS	D	380	45.922	80.912	198.838	1.00	182.01
	3731	CE	LYS	D	380	46.121	79.480	198.365	1.00	174.42
50	3732	NZ	LYS	D	380	47.562	79.099	198.345	1.00	158.73
	3733	C	LYS	D	380	42.737	84.654	199.854	1.00	146.29
	3734	O	LYS	D	380	43.016	85.582	199.096	1.00	155.06
	3735	N	PRO	D	381	42.360	84.863	201.126	1.00	140.56
	3736	CD	PRO	D	381	41.968	83.800	202.069	1.00	154.32
55	3737	CA	PRO	D	381	42.240	86.184	201.757	1.00	132.74

	3738	CB	PRO	D	381	42.074	85.834	203.231	1.00	144.55
	3739	CG	PRO	D	381	41.264	84.578	203.163	1.00	138.88
	3740	C	PRO	D	381	43.428	87.119	201.507	1.00	118.02
	3741	O	PRO	D	381	44.490	86.675	201.074	1.00	99.94
5	3742	N	VAL	D	382	43.239	88.410	201.793	1.00	105.18
	3743	CA	VAL	D	382	44.279	89.429	201.584	1.00	80.19
	3744	CB	VAL	D	382	43.901	90.375	200.458	1.00	64.06
	3745	CG1	VAL	D	382	43.890	89.629	199.140	1.00	134.59
	3746	CG2	VAL	D	382	42.530	90.963	200.739	1.00	87.60
10	3747	C	VAL	D	382	44.553	90.305	202.791	1.00	102.12
	3748	O	VAL	D	382	43.654	90.583	203.581	1.00	116.29
	3749	N	ASN	D	383	45.796	90.764	202.913	1.00	100.94
	3750	CA	ASN	D	383	46.189	91.618	204.033	1.00	127.59
	3751	CB	ASN	D	383	47.694	91.910	203.982	1.00	137.48
15	3752	CG	ASN	D	383	48.543	90.699	204.346	1.00	150.77
	3753	OD1	ASN	D	383	49.767	90.707	204.178	1.00	132.07
	3754	ND2	ASN	D	383	47.897	89.654	204.857	1.00	146.01
	3755	C	ASN	D	383	45.411	92.928	203.998	1.00	88.67
	3756	O	ASN	D	383	44.731	93.223	203.021	1.00	96.54
20	3757	N	HIS	D	384	45.510	93.708	205.068	1.00	90.17
	3758	CA	HIS	D	384	44.810	94.985	205.142	1.00	76.61
	3759	CB	HIS	D	384	44.747	95.464	206.594	1.00	88.84
	3760	CG	HIS	D	384	43.971	94.546	207.492	1.00	115.42
	3761	CD2	HIS	D	384	44.367	93.491	208.244	1.00	119.90
25	3762	ND1	HIS	D	384	42.602	94.630	207.639	1.00	93.91
	3763	CE1	HIS	D	384	42.189	93.665	208.443	1.00	115.01
	3764	NE2	HIS	D	384	43.239	92.960	208.823	1.00	139.25
	3765	C	HIS	D	384	45.538	95.996	204.281	1.00	71.38
	3766	O	HIS	D	384	46.757	96.000	204.219	1.00	48.03
30	3767	N	SER	D	385	44.787	96.859	203.617	1.00	81.66
	3768	CA	SER	D	385	45.396	97.845	202.748	1.00	36.20
	3769	CB	SER	D	385	44.638	97.893	201.424	1.00	66.21
	3770	OG	SER	D	385	43.265	98.161	201.638	1.00	99.18
	3771	C	SER	D	385	45.467	99.247	203.338	1.00	61.33
35	3772	O	SER	D	385	44.928	99.529	204.404	1.00	72.76
	3773	N	THR	D	386	46.130	100.119	202.601	1.00	38.22
	3774	CA	THR	D	386	46.341	101.507	202.949	1.00	30.42
	3775	CB	THR	D	386	47.810	101.868	202.631	1.00	78.59
	3776	OG1	THR	D	386	48.625	101.545	203.761	1.00	109.39
40	3777	CG2	THR	D	386	47.973	103.333	202.247	1.00	82.78
	3778	C	THR	D	386	45.416	102.332	202.086	1.00	55.16
	3779	O	THR	D	386	44.858	101.819	201.124	1.00	85.45
	3780	N	ARG	D	387	45.240	103.608	202.412	1.00	60.12
	3781	CA	ARG	D	387	44.399	104.459	201.569	1.00	57.26
45	3782	CB	ARG	D	387	42.956	104.032	201.709	1.00	45.25
	3783	CG	ARG	D	387	41.990	104.919	200.996	1.00	58.55
	3784	CD	ARG	D	387	40.661	104.219	200.838	1.00	62.37
	3785	NE	ARG	D	387	39.669	105.097	200.233	1.00	75.16
	3786	CZ	ARG	D	387	38.472	104.694	199.827	1.00	113.22
50	3787	NH1	ARG	D	387	38.125	103.418	199.965	1.00	105.83
	3788	NH2	ARG	D	387	37.627	105.564	199.282	1.00	88.31
	3789	C	ARG	D	387	44.528	105.952	201.834	1.00	49.54
	3790	O	ARG	D	387	44.421	106.373	202.977	1.00	74.17
	3791	N	LYS	D	388	44.759	106.743	200.784	1.00	14.61
55	3792	CA	LYS	D	388	44.909	108.195	200.915	1.00	49.64

	3793	CB	LYS	D	388	46.349	108.672	200.653	1.00	19.49
	3794	CG	LYS	D	388	47.490	107.749	201.074	1.00	148.66
	3795	CD	LYS	D	388	48.839	108.366	200.675	1.00	145.63
	3796	CE	LYS	D	388	50.016	107.483	201.069	1.00	169.40
5	3797	NZ	LYS	D	388	51.321	108.173	200.844	1.00	149.37
	3798	C	LYS	D	388	44.068	108.854	199.854	1.00	40.50
	3799	O	LYS	D	388	44.011	108.358	198.735	1.00	60.66
	3800	N	GLU	D	389	43.425	109.971	200.183	1.00	34.31
	3801	CA	GLU	D	389	42.645	110.713	199.183	1.00	51.61
10	3802	CB	GLU	D	389	41.143	110.672	199.478	1.00	15.19
	3803	CG	GLU	D	389	40.520	109.280	199.334	1.00	140.73
	3804	CD	GLU	D	389	39.070	109.211	199.796	1.00	168.49
	3805	OE1	GLU	D	389	38.263	110.060	199.354	1.00	149.55
	3806	OE2	GLU	D	389	38.741	108.300	200.594	1.00	151.07
15	3807	C	GLU	D	389	43.118	112.159	199.147	1.00	49.41
	3808	O	GLU	D	389	42.719	112.969	199.973	1.00	85.28
	3809	N	GLU	D	390	43.966	112.478	198.178	1.00	36.48
	3810	CA	GLU	D	390	44.525	113.817	198.052	1.00	75.79
	3811	CB	GLU	D	390	46.005	113.748	197.638	1.00	105.75
20	3812	CG	GLU	D	390	46.901	112.828	198.462	1.00	149.81
	3813	CD	GLU	D	390	48.363	112.896	198.028	1.00	166.87
	3814	OE1	GLU	D	390	48.638	112.760	196.814	1.00	167.85
	3815	OE2	GLU	D	390	49.237	113.080	198.903	1.00	158.75
	3816	C	GLU	D	390	43.826	114.727	197.055	1.00	24.22
25	3817	O	GLU	D	390	43.939	114.519	195.855	1.00	71.23
	3818	N	LYS	D	391	43.126	115.746	197.535	1.00	39.14
	3819	CA	LYS	D	391	42.485	116.689	196.620	1.00	57.00
	3820	CB	LYS	D	391	41.731	117.794	197.388	1.00	45.82
	3821	CG	LYS	D	391	41.324	118.992	196.519	1.00	82.77
30	3822	CD	LYS	D	391	41.375	120.325	197.271	1.00	142.55
	3823	CE	LYS	D	391	40.285	120.453	198.331	1.00	170.58
	3824	NZ	LYS	D	391	40.286	121.807	198.979	1.00	121.90
	3825	C	LYS	D	391	43.652	117.317	195.856	1.00	48.81
	3826	O	LYS	D	391	44.550	117.872	196.476	1.00	51.69
35	3827	N	GLN	D	392	43.649	117.218	194.526	1.00	65.02
	3828	CA	GLN	D	392	44.730	117.787	193.725	1.00	59.17
	3829	CB	GLN	D	392	44.920	116.991	192.448	1.00	65.61
	3830	CG	GLN	D	392	45.169	115.537	192.684	1.00	54.54
	3831	CD	GLN	D	392	46.454	115.307	193.399	1.00	38.88
40	3832	OE1	GLN	D	392	46.604	115.681	194.556	1.00	126.60
	3833	NE2	GLN	D	392	47.412	114.693	192.712	1.00	107.57
	3834	C	GLN	D	392	44.461	119.237	193.368	1.00	88.60
	3835	O	GLN	D	392	43.348	119.743	193.559	1.00	64.57
	3836	N	ARG	D	393	45.487	119.896	192.835	1.00	88.23
45	3837	CA	ARG	D	393	45.381	121.299	192.463	1.00	103.72
	3838	CB	ARG	D	393	46.747	121.855	192.045	1.00	134.66
	3839	CG	ARG	D	393	46.697	123.320	191.590	1.00	159.94
	3840	CD	ARG	D	393	47.397	124.271	192.559	1.00	160.67
	3841	NE	ARG	D	393	48.846	124.077	192.564	1.00	168.47
50	3842	CZ	ARG	D	393	49.702	124.859	193.212	1.00	172.58
	3843	NH1	ARG	D	393	49.257	125.894	193.913	1.00	174.62
	3844	NH2	ARG	D	393	51.004	124.606	193.160	1.00	174.39
	3845	C	ARG	D	393	44.382	121.561	191.351	1.00	83.46
	3846	O	ARG	D	393	43.633	122.543	191.414	1.00	96.92
55	3847	N	ASN	D	394	44.357	120.694	190.338	1.00	93.61

	3848	CA	ASN	D	394	43.437	120.897	189.219	1.00	95.98
	3849	CB	ASN	D	394	43.924	120.138	187.969	1.00	83.40
	3850	CG	ASN	D	394	43.957	118.632	188.154	1.00	48.87
	3851	OD1	ASN	D	394	43.110	118.070	188.828	1.00	66.78
	3852	ND2	ASN	D	394	44.927	117.982	187.516	1.00	75.04
	3853	C	ASN	D	394	41.952	120.583	189.479	1.00	59.45
	3854	O	ASN	D	394	41.227	120.189	188.572	1.00	59.33
	3855	N	GLY	D	395	41.494	120.775	190.710	1.00	79.33
	3856	CA	GLY	D	395	40.099	120.509	191.008	1.00	71.67
	3857	C	GLY	D	395	39.724	119.038	191.108	1.00	59.87
	3858	O	GLY	D	395	38.677	118.700	191.669	1.00	74.71
	3859	N	THR	D	396	40.564	118.157	190.574	1.00	62.74
	3860	CA	THR	D	396	40.274	116.730	190.626	1.00	61.60
	3861	CB	THR	D	396	41.206	115.932	189.705	1.00	47.87
	3862	OG1	THR	D	396	40.702	114.600	189.558	1.00	156.72
	3863	CG2	THR	D	396	42.599	115.848	190.305	1.00	112.24
	3864	C	THR	D	396	40.436	116.198	192.048	1.00	53.86
	3865	O	THR	D	396	40.495	116.964	193.001	1.00	71.70
	3866	N	LEU	D	397	40.520	114.878	192.171	1.00	45.95
	3867	CA	LEU	D	397	40.655	114.203	193.454	1.00	53.38
	3868	CB	LEU	D	397	39.281	114.097	194.110	1.00	59.95
	3869	CG	LEU	D	397	39.121	113.074	195.221	1.00	55.86
	3870	CD1	LEU	D	397	40.080	113.397	196.345	1.00	111.38
	3871	CD2	LEU	D	397	37.685	113.061	195.710	1.00	106.37
	3872	C	LEU	D	397	41.232	112.809	193.198	1.00	50.48
	3873	O	LEU	D	397	40.675	112.039	192.417	1.00	62.36
	3874	N	THR	D	398	42.337	112.493	193.868	1.00	40.39
	3875	CA	THR	D	398	43.020	111.224	193.706	1.00	21.97
	3876	CB	THR	D	398	44.512	111.441	193.543	1.00	25.83
	3877	OG1	THR	D	398	44.756	112.125	192.315	1.00	66.94
	3878	CG2	THR	D	398	45.246	110.136	193.527	1.00	67.01
	3879	C	THR	D	398	42.844	110.303	194.865	1.00	24.03
	3880	O	THR	D	398	42.586	110.737	195.973	1.00	59.86
	3881	N	VAL	D	399	43.008	109.015	194.602	1.00	37.39
	3882	CA	VAL	D	399	42.909	107.980	195.628	1.00	37.07
	3883	CB	VAL	D	399	41.574	107.254	195.564	1.00	32.64
	3884	CG1	VAL	D	399	41.609	106.041	196.480	1.00	32.87
	3885	CG2	VAL	D	399	40.476	108.176	195.946	1.00	28.21
	3886	C	VAL	D	399	43.973	106.932	195.385	1.00	41.18
	3887	O	VAL	D	399	44.031	106.372	194.293	1.00	45.84
	3888	N	THR	D	400	44.818	106.664	196.375	1.00	50.23
	3889	CA	THR	D	400	45.834	105.625	196.202	1.00	38.12
	3890	CB	THR	D	400	47.270	106.128	196.319	1.00	43.92
	3891	OG1	THR	D	400	47.494	106.558	197.655	1.00	69.44
	3892	CG2	THR	D	400	47.526	107.280	195.375	1.00	45.17
	3893	C	THR	D	400	45.648	104.626	197.309	1.00	35.51
	3894	O	THR	D	400	45.223	104.968	198.404	1.00	64.95
	3895	N	SER	D	401	45.969	103.382	197.016	1.00	42.58
	3896	CA	SER	D	401	45.840	102.318	197.990	1.00	42.11
	3897	CB	SER	D	401	44.515	101.584	197.833	1.00	59.45
	3898	OG	SER	D	401	44.482	100.421	198.643	1.00	51.13
	3899	C	SER	D	401	46.946	101.344	197.735	1.00	49.43
	3900	O	SER	D	401	47.042	100.807	196.641	1.00	49.62
	3901	N	THR	D	402	47.779	101.118	198.742	1.00	72.73
	3902	CA	THR	D	402	48.894	100.196	198.624	1.00	50.60

	3903	CB	THR	D	402	50.150	100.813	199.187	1.00	50.34
	3904	OG1	THR	D	402	50.322	102.117	198.630	1.00	61.02
	3905	CG2	THR	D	402	51.345	99.975	198.836	1.00	108.37
	3906	C	THR	D	402	48.571	98.928	199.394	1.00	59.31
5	3907	O	THR	D	402	47.951	98.978	200.447	1.00	73.63
	3908	N	LEU	D	403	48.995	97.790	198.872	1.00	60.48
	3909	CA	LEU	D	403	48.701	96.520	199.510	1.00	51.40
	3910	CB	LEU	D	403	47.648	95.785	198.689	1.00	60.86
	3911	CG	LEU	D	403	47.239	94.398	199.166	1.00	71.08
10	3912	CD1	LEU	D	403	46.519	94.506	200.492	1.00	115.39
	3913	CD2	LEU	D	403	46.339	93.757	198.140	1.00	75.16
	3914	C	LEU	D	403	49.919	95.624	199.684	1.00	86.73
	3915	O	LEU	D	403	50.684	95.411	198.741	1.00	48.79
	3916	N	PRO	D	404	50.113	95.090	200.901	1.00	45.77
15	3917	CD	PRO	D	404	49.349	95.460	202.098	1.00	72.52
	3918	CA	PRO	D	404	51.215	94.203	201.270	1.00	60.92
	3919	CB	PRO	D	404	51.070	94.080	202.784	1.00	110.61
	3920	CG	PRO	D	404	50.390	95.345	203.168	1.00	84.70
	3921	C	PRO	D	404	51.030	92.861	200.573	1.00	78.31
20	3922	O	PRO	D	404	49.926	92.321	200.528	1.00	62.25
	3923	N	VAL	D	405	52.116	92.304	200.055	1.00	85.38
	3924	CA	VAL	D	405	52.015	91.056	199.330	1.00	72.08
	3925	CB	VAL	D	405	52.032	91.358	197.832	1.00	42.37
	3926	CG1	VAL	D	405	53.051	90.497	197.120	1.00	129.72
25	3927	CG2	VAL	D	405	50.651	91.145	197.266	1.00	97.10
	3928	C	VAL	D	405	53.063	90.002	199.661	1.00	107.38
	3929	O	VAL	D	405	54.263	90.289	199.721	1.00	92.57
	3930	N	GLY	D	406	52.584	88.772	199.849	1.00	74.73
	3931	CA	GLY	D	406	53.459	87.656	200.171	1.00	128.36
30	3932	C	GLY	D	406	54.503	87.396	199.084	1.00	128.26
	3933	O	GLY	D	406	54.170	86.932	197.995	1.00	94.96
	3934	N	THR	D	407	55.763	87.675	199.410	1.00	145.41
	3935	CA	THR	D	407	56.880	87.505	198.508	1.00	103.78
	3936	CB	THR	D	407	58.220	87.513	199.231	1.00	128.76
35	3937	OG1	THR	D	407	58.109	88.244	200.452	1.00	153.49
	3938	CG2	THR	D	407	59.289	88.139	198.329	1.00	97.34
	3939	C	THR	D	407	56.852	86.189	197.741	1.00	107.15
	3940	O	THR	D	407	57.225	86.126	196.572	1.00	95.02
	3941	N	ARG	D	408	56.441	85.123	198.408	1.00	126.42
40	3942	CA	ARG	D	408	56.399	83.820	197.772	1.00	134.10
	3943	CB	ARG	D	408	56.112	82.750	198.816	1.00	151.42
	3944	CG	ARG	D	408	57.188	82.649	199.914	1.00	177.48
	3945	CD	ARG	D	408	57.344	83.945	200.730	1.00	172.46
	3946	NE	ARG	D	408	56.196	84.229	201.588	1.00	159.11
45	3947	CZ	ARG	D	408	56.079	85.320	202.337	1.00	143.95
	3948	NH1	ARG	D	408	57.038	86.240	202.332	1.00	95.33
	3949	NH2	ARG	D	408	55.013	85.480	203.107	1.00	128.49
	3950	C	ARG	D	408	55.302	83.805	196.723	1.00	126.54
	3951	O	ARG	D	408	55.556	83.753	195.505	1.00	112.58
50	3952	N	ASP	D	409	54.070	83.869	197.211	1.00	115.25
	3953	CA	ASP	D	409	52.874	83.849	196.382	1.00	99.87
	3954	CB	ASP	D	409	51.731	84.516	197.160	1.00	106.74
	3955	CG	ASP	D	409	51.541	83.939	198.559	1.00	132.42
	3956	OD1	ASP	D	409	51.021	82.808	198.688	1.00	129.76
55	3957	OD2	ASP	D	409	51.909	84.625	199.539	1.00	112.17

	3958	C	ASP	D	409	53.053	84.546	195.032	1.00	89.51
	3959	O	ASP	D	409	52.675	84.000	193.990	1.00	130.58
	3960	N	TRP	D	410	53.622	85.749	195.061	1.00	75.82
	3961	CA	TRP	D	410	53.836	86.534	193.853	1.00	67.87
	3962	CB	TRP	D	410	54.487	87.863	194.209	1.00	73.93
	3963	CG	TRP	D	410	54.924	88.660	193.025	1.00	51.99
	3964	CD2	TRP	D	410	54.138	89.608	192.297	1.00	89.75
	3965	CE2	TRP	D	410	54.954	90.123	191.266	1.00	74.90
	3966	CE3	TRP	D	410	52.822	90.071	192.416	1.00	51.02
	3967	CD1	TRP	D	410	56.145	88.636	192.423	1.00	101.45
	3968	NE1	TRP	D	410	56.174	89.515	191.365	1.00	51.04
	3969	CZ2	TRP	D	410	54.498	91.083	190.357	1.00	99.21
	3970	CZ3	TRP	D	410	52.369	91.020	191.518	1.00	50.44
	3971	CH2	TRP	D	410	53.208	91.520	190.496	1.00	72.30
	3972	C	TRP	D	410	54.684	85.829	192.825	1.00	97.87
	3973	O	TRP	D	410	54.246	85.630	191.693	1.00	127.37
	3974	N	ILE	D	411	55.900	85.458	193.215	1.00	107.01
	3975	CA	ILE	D	411	56.807	84.797	192.283	1.00	114.82
	3976	CB	ILE	D	411	58.125	84.422	192.943	1.00	90.18
	3977	CG2	ILE	D	411	59.219	84.374	191.890	1.00	113.38
	3978	CG1	ILE	D	411	58.504	85.477	193.973	1.00	122.60
	3979	CD1	ILE	D	411	59.713	85.112	194.782	1.00	160.55
	3980	C	ILE	D	411	56.182	83.539	191.713	1.00	131.40
	3981	O	ILE	D	411	56.470	83.146	190.585	1.00	115.52
	3982	N	GLU	D	412	55.322	82.903	192.497	1.00	92.44
	3983	CA	GLU	D	412	54.655	81.704	192.031	1.00	108.96
	3984	CB	GLU	D	412	54.287	80.823	193.216	1.00	133.49
	3985	CG	GLU	D	412	55.489	80.102	193.793	1.00	154.48
	3986	CD	GLU	D	412	55.112	79.134	194.888	1.00	184.63
	3987	OE1	GLU	D	412	54.194	78.315	194.668	1.00	187.73
	3988	OE2	GLU	D	412	55.738	79.187	195.967	1.00	191.09
	3989	C	GLU	D	412	53.428	81.997	191.162	1.00	137.18
	3990	O	GLU	D	412	52.457	81.236	191.149	1.00	129.46
	3991	N	GLY	D	413	53.485	83.118	190.446	1.00	164.33
	3992	CA	GLY	D	413	52.417	83.501	189.535	1.00	162.77
	3993	C	GLY	D	413	51.059	83.957	190.041	1.00	141.45
	3994	O	GLY	D	413	50.144	84.149	189.237	1.00	136.83
	3995	N	GLU	D	414	50.903	84.135	191.347	1.00	129.17
	3996	CA	GLU	D	414	49.620	84.580	191.869	1.00	99.45
	3997	CB	GLU	D	414	49.731	84.925	193.349	1.00	110.96
	3998	CG	GLU	D	414	48.471	85.542	193.936	1.00	90.67
	3999	CD	GLU	D	414	47.256	84.634	193.834	1.00	94.32
	4000	OE1	GLU	D	414	46.758	84.399	192.709	1.00	112.62
	4001	OE2	GLU	D	414	46.802	84.152	194.891	1.00	91.31
	4002	C	GLU	D	414	49.146	85.803	191.098	1.00	100.87
	4003	O	GLU	D	414	49.917	86.424	190.368	1.00	107.15
	4004	N	THR	D	415	47.876	86.149	191.266	1.00	111.06
	4005	CA	THR	D	415	47.303	87.291	190.574	1.00	112.82
	4006	CB	THR	D	415	46.590	86.825	189.295	1.00	119.50
	4007	OG1	THR	D	415	45.583	87.773	188.933	1.00	115.11
	4008	CG2	THR	D	415	45.993	85.452	189.487	1.00	150.67
	4009	C	THR	D	415	46.348	88.115	191.442	1.00	127.64
	4010	O	THR	D	415	45.360	87.595	191.982	1.00	91.30
	4011	N	TYR	D	416	46.664	89.407	191.559	1.00	114.78
	4012	CA	TYR	D	416	45.899	90.360	192.366	1.00	69.47

	4013	CB	TYR	D	416	46.846	91.150	193.276	1.00	76.73
	4014	CG	TYR	D	416	47.732	90.297	194.155	1.00	89.68
	4015	CD1	TYR	D	416	48.988	89.875	193.724	1.00	115.56
	4016	CE1	TYR	D	416	49.787	89.049	194.524	1.00	52.64
5	4017	CD2	TYR	D	416	47.298	89.877	195.406	1.00	74.22
	4018	CE2	TYR	D	416	48.086	89.054	196.210	1.00	65.75
	4019	CZ	TYR	D	416	49.321	88.645	195.766	1.00	79.16
	4020	OH	TYR	D	416	50.081	87.831	196.571	1.00	157.74
	4021	C	TYR	D	416	45.089	91.342	191.521	1.00	92.20
10	4022	O	TYR	D	416	45.521	91.745	190.438	1.00	69.13
	4023	N	GLN	D	417	43.931	91.752	192.037	1.00	67.36
	4024	CA	GLN	D	417	43.050	92.668	191.319	1.00	48.33
	4025	CB	GLN	D	417	41.897	91.876	190.709	1.00	124.19
	4026	CG	GLN	D	417	41.057	92.649	189.718	1.00	145.26
15	4027	CD	GLN	D	417	39.854	91.857	189.256	1.00	138.49
	4028	OE1	GLN	D	417	38.942	91.590	190.037	1.00	121.32
	4029	NE2	GLN	D	417	39.848	91.469	187.985	1.00	129.85
	4030	C	GLN	D	417	42.484	93.795	192.191	1.00	57.83
	4031	O	GLN	D	417	42.091	93.579	193.338	1.00	77.99
20	4032	N	CYS	D	418	42.426	94.992	191.614	1.00	66.84
	4033	CA	CYS	D	418	41.930	96.191	192.286	1.00	48.93
	4034	C	CYS	D	418	40.585	96.549	191.670	1.00	61.50
	4035	O	CYS	D	418	40.496	96.739	190.465	1.00	67.84
	4036	CB	CYS	D	418	42.927	97.336	192.079	1.00	66.08
25	4037	SG	CYS	D	418	42.483	98.904	192.868	1.00	95.99
	4038	N	ARG	D	419	39.541	96.638	192.490	1.00	50.79
	4039	CA	ARG	D	419	38.201	96.969	191.992	1.00	30.24
	4040	CB	ARG	D	419	37.226	95.822	192.284	1.00	108.73
	4041	CG	ARG	D	419	35.835	96.025	191.697	1.00	188.65
30	4042	CD	ARG	D	419	34.860	94.941	192.125	1.00	228.92
	4043	NE	ARG	D	419	33.561	95.099	191.473	1.00	243.94
	4044	CZ	ARG	D	419	32.495	94.354	191.738	1.00	230.39
	4045	NH1	ARG	D	419	32.566	93.394	192.649	1.00	220.71
	4046	NH2	ARG	D	419	31.359	94.565	191.090	1.00	214.39
35	4047	C	ARG	D	419	37.661	98.255	192.610	1.00	69.76
	4048	O	ARG	D	419	37.299	98.287	193.797	1.00	59.29
	4049	N	VAL	D	420	37.597	99.315	191.809	1.00	18.00
	4050	CA	VAL	D	420	37.074	100.578	192.324	1.00	56.50
	4051	CB	VAL	D	420	37.934	101.774	191.866	1.00	52.22
40	4052	CG1	VAL	D	420	39.318	101.315	191.544	1.00	42.61
	4053	CG2	VAL	D	420	37.327	102.441	190.689	1.00	35.59
	4054	C	VAL	D	420	35.665	100.745	191.782	1.00	35.00
	4055	O	VAL	D	420	35.385	100.297	190.700	1.00	37.99
	4056	N	THR	D	421	34.772	101.395	192.502	1.00	56.57
45	4057	CA	THR	D	421	33.425	101.562	191.982	1.00	23.71
	4058	CB	THR	D	421	32.465	100.554	192.642	1.00	45.48
	4059	OG1	THR	D	421	32.418	100.794	194.052	1.00	67.88
	4060	CG2	THR	D	421	32.941	99.141	192.431	1.00	34.10
	4061	C	THR	D	421	32.981	102.971	192.327	1.00	45.43
50	4062	O	THR	D	421	33.240	103.446	193.427	1.00	48.61
	4063	N	HIS	D	422	32.334	103.649	191.389	1.00	43.04
	4064	CA	HIS	D	422	31.840	105.009	191.627	1.00	50.66
	4065	CB	HIS	D	422	32.559	106.002	190.718	1.00	14.59
	4066	CG	HIS	D	422	32.154	107.422	190.931	1.00	21.53
55	4067	CD2	HIS	D	422	32.698	108.580	190.485	1.00	65.88

	4068	ND1	HIS	D	422	31.052	107.779	191.675	1.00	53.72
	4069	CE1	HIS	D	422	30.935	109.095	191.681	1.00	114.73
	4070	NE2	HIS	D	422	31.922	109.606	190.966	1.00	87.07
	4071	C	HIS	D	422	30.344	105.008	191.319	1.00	73.12
5	4072	O	HIS	D	422	29.920	104.610	190.236	1.00	67.37
	4073	N	PRO	D	423	29.523	105.465	192.265	1.00	58.08
	4074	CD	PRO	D	423	29.888	106.227	193.469	1.00	54.31
	4075	CA	PRO	D	423	28.076	105.492	192.059	1.00	71.43
	4076	CB	PRO	D	423	27.608	106.488	193.108	1.00	46.51
10	4077	CG	PRO	D	423	28.588	106.285	194.211	1.00	82.86
	4078	C	PRO	D	423	27.619	105.884	190.654	1.00	63.28
	4079	O	PRO	D	423	26.833	105.173	190.028	1.00	81.37
	4080	N	HIS	D	424	28.123	107.005	190.157	1.00	34.90
	4081	CA	HIS	D	424	27.730	107.502	188.848	1.00	59.77
15	4082	CB	HIS	D	424	28.010	108.999	188.754	1.00	37.61
	4083	CG	HIS	D	424	27.748	109.743	190.019	1.00	60.94
	4084	CD2	HIS	D	424	27.244	109.336	191.207	1.00	98.42
	4085	ND1	HIS	D	424	28.068	111.072	190.174	1.00	78.59
	4086	CE1	HIS	D	424	27.778	111.452	191.406	1.00	152.64
20	4087	NE2	HIS	D	424	27.277	110.417	192.054	1.00	152.52
	4088	C	HIS	D	424	28.388	106.814	187.654	1.00	36.89
	4089	O	HIS	D	424	28.568	107.433	186.612	1.00	54.52
	4090	N	LEU	D	425	28.758	105.548	187.776	1.00	21.15
	4091	CA	LEU	D	425	29.371	104.884	186.632	1.00	37.06
25	4092	CB	LEU	D	425	30.857	104.611	186.893	1.00	56.98
	4093	CG	LEU	D	425	31.771	105.825	187.067	1.00	23.50
	4094	CD1	LEU	D	425	33.179	105.368	187.366	1.00	58.60
	4095	CD2	LEU	D	425	31.746	106.677	185.827	1.00	24.67
	4096	C	LEU	D	425	28.680	103.584	186.237	1.00	31.46
30	4097	O	LEU	D	425	28.161	102.858	187.077	1.00	64.74
	4098	N	PRO	D	426	28.660	103.287	184.936	1.00	23.81
	4099	CD	PRO	D	426	29.067	104.203	183.862	1.00	71.59
	4100	CA	PRO	D	426	28.053	102.088	184.376	1.00	41.36
	4101	CB	PRO	D	426	28.260	102.281	182.885	1.00	29.87
35	4102	CG	PRO	D	426	28.215	103.739	182.734	1.00	66.78
	4103	C	PRO	D	426	28.735	100.834	184.912	1.00	26.52
	4104	O	PRO	D	426	28.315	100.289	185.916	1.00	55.27
	4105	N	ARG	D	427	29.785	100.369	184.249	1.00	73.53
	4106	CA	ARG	D	427	30.472	99.182	184.725	1.00	63.70
40	4107	CB	ARG	D	427	31.083	98.404	183.541	1.00	62.24
	4108	CG	ARG	D	427	30.616	96.941	183.493	1.00	74.02
	4109	CD	ARG	D	427	31.214	96.127	182.354	1.00	70.65
	4110	NE	ARG	D	427	31.336	94.711	182.718	1.00	159.98
	4111	CZ	ARG	D	427	31.878	93.762	181.953	1.00	164.46
45	4112	NH1	ARG	D	427	32.363	94.046	180.749	1.00	124.37
	4113	NH2	ARG	D	427	31.951	92.516	182.405	1.00	133.62
	4114	C	ARG	D	427	31.532	99.618	185.751	1.00	86.41
	4115	O	ARG	D	427	31.880	100.800	185.828	1.00	47.25
	4116	N	ALA	D	428	32.013	98.674	186.559	1.00	93.41
50	4117	CA	ALA	D	428	33.005	98.970	187.595	1.00	41.66
	4118	CB	ALA	D	428	32.956	97.912	188.669	1.00	102.75
	4119	C	ALA	D	428	34.400	99.058	187.028	1.00	45.06
	4120	O	ALA	D	428	34.674	98.543	185.958	1.00	75.62
	4121	N	LEU	D	429	35.291	99.721	187.744	1.00	66.10
55	4122	CA	LEU	D	429	36.641	99.848	187.242	1.00	43.45

	4123	CB	LEU	D	429	37.222	101.217	187.556	1.00	34.38
	4124	CG	LEU	D	429	37.745	101.978	186.364	1.00	66.23
	4125	CD1	LEU	D	429	38.458	103.214	186.845	1.00	46.80
	4126	CD2	LEU	D	429	38.672	101.084	185.569	1.00	115.61
5	4127	C	LEU	D	429	37.484	98.785	187.887	1.00	54.85
	4128	O	LEU	D	429	37.496	98.631	189.117	1.00	59.59
	4129	N	MET	D	430	38.184	98.040	187.043	1.00	47.43
	4130	CA	MET	D	430	39.057	96.962	187.494	1.00	53.01
	4131	CB	MET	D	430	38.412	95.594	187.284	1.00	40.35
10	4132	CG	MET	D	430	37.179	95.375	188.128	1.00	77.82
	4133	SD	MET	D	430	36.525	93.713	187.975	1.00	126.20
	4134	CE	MET	D	430	35.574	93.859	186.419	1.00	161.71
	4135	C	MET	D	430	40.366	96.986	186.745	1.00	63.35
	4136	O	MET	D	430	40.448	97.480	185.612	1.00	42.39
15	4137	N	ARG	D	431	41.392	96.466	187.407	1.00	36.33
	4138	CA	ARG	D	431	42.719	96.379	186.841	1.00	58.15
	4139	CB	ARG	D	431	43.464	97.696	186.993	1.00	27.19
	4140	CG	ARG	D	431	42.683	98.900	186.503	1.00	33.53
	4141	CD	ARG	D	431	43.552	99.896	185.806	1.00	43.03
20	4142	NE	ARG	D	431	43.438	99.788	184.355	1.00	95.31
	4143	CZ	ARG	D	431	42.328	100.067	183.679	1.00	104.17
	4144	NH1	ARG	D	431	41.245	100.468	184.330	1.00	37.36
	4145	NH2	ARG	D	431	42.300	99.949	182.355	1.00	165.84
	4146	C	ARG	D	431	43.363	95.299	187.666	1.00	67.38
25	4147	O	ARG	D	431	43.050	95.151	188.839	1.00	56.89
	4148	N	SER	D	432	44.240	94.527	187.046	1.00	77.67
	4149	CA	SER	D	432	44.897	93.431	187.734	1.00	64.82
	4150	CB	SER	D	432	44.192	92.118	187.410	1.00	56.74
	4151	OG	SER	D	432	44.290	91.820	186.027	1.00	99.74
30	4152	C	SER	D	432	46.343	93.350	187.291	1.00	94.30
	4153	O	SER	D	432	46.754	94.039	186.355	1.00	64.60
	4154	N	THR	D	433	47.112	92.507	187.969	1.00	73.10
	4155	CA	THR	D	433	48.519	92.339	187.647	1.00	82.03
	4156	CB	THR	D	433	49.341	93.538	188.076	1.00	73.97
35	4157	OG1	THR	D	433	50.696	93.368	187.640	1.00	108.43
	4158	CG2	THR	D	433	49.314	93.664	189.589	1.00	50.90
	4159	C	THR	D	433	49.110	91.140	188.340	1.00	97.97
	4160	O	THR	D	433	48.687	90.772	189.450	1.00	54.76
	4161	N	THR	D	434	50.101	90.543	187.673	1.00	88.14
40	4162	CA	THR	D	434	50.835	89.377	188.176	1.00	61.31
	4163	CB	THR	D	434	50.212	88.050	187.757	1.00	73.67
	4164	OG1	THR	D	434	50.604	87.723	186.414	1.00	136.86
	4165	CG2	THR	D	434	48.713	88.120	187.813	1.00	65.49
	4166	C	THR	D	434	52.219	89.389	187.548	1.00	93.47
45	4167	O	THR	D	434	52.500	90.185	186.661	1.00	68.59
	4168	N	LYS	D	435	53.052	88.481	188.041	1.00	104.82
	4169	CA	LYS	D	435	54.425	88.280	187.620	1.00	97.19
	4170	CB	LYS	D	435	54.913	86.952	188.190	1.00	108.47
	4171	CG	LYS	D	435	56.289	86.406	187.805	1.00	156.78
50	4172	CD	LYS	D	435	56.494	85.099	188.627	1.00	153.33
	4173	CE	LYS	D	435	57.777	84.278	188.369	1.00	171.23
	4174	NZ	LYS	D	435	57.958	83.976	186.919	1.00	182.18
	4175	C	LYS	D	435	54.554	88.263	186.100	1.00	93.46
	4176	O	LYS	D	435	53.814	87.555	185.412	1.00	120.14
55	4177	N	THR	D	436	55.489	89.042	185.566	1.00	71.73

	4178	CA	THR	D	436	55.677	89.079	184.118	1.00	82.60
	4179	CB	THR	D	436	56.715	90.111	183.748	1.00	75.56
	4180	OG1	THR	D	436	56.400	91.352	184.383	1.00	131.33
	4181	CG2	THR	D	436	56.746	90.317	182.254	1.00	83.66
5	4182	C	THR	D	436	56.132	87.718	183.594	1.00	127.18
	4183	O	THR	D	436	56.943	87.046	184.224	1.00	131.75
	4184	N	SER	D	437	55.651	87.344	182.413	1.00	129.98
	4185	CA	SER	D	437	55.976	86.043	181.824	1.00	150.36
	4186	CB	SER	D	437	54.732	85.467	181.140	1.00	156.11
10	4187	OG	SER	D	437	54.249	86.345	180.132	1.00	150.74
	4188	C	SER	D	437	57.136	86.032	180.844	1.00	145.33
	4189	O	SER	D	437	57.791	87.049	180.633	1.00	128.92
	4190	N	GLY	D	438	57.385	84.861	180.261	1.00	143.82
	4191	CA	GLY	D	438	58.455	84.708	179.289	1.00	129.59
15	4192	C	GLY	D	438	59.692	83.989	179.804	1.00	109.80
	4193	O	GLY	D	438	59.641	83.339	180.849	1.00	90.90
	4194	N	PRO	D	439	60.814	84.057	179.066	1.00	96.86
	4195	CD	PRO	D	439	60.853	84.528	177.672	1.00	102.41
	4196	CA	PRO	D	439	62.088	83.431	179.427	1.00	112.86
20	4197	CB	PRO	D	439	62.754	83.224	178.079	1.00	143.69
	4198	CG	PRO	D	439	62.322	84.442	177.338	1.00	120.60
	4199	C	PRO	D	439	62.861	84.406	180.312	1.00	120.63
	4200	O	PRO	D	439	62.881	85.600	180.044	1.00	129.73
	4201	N	ARG	D	440	63.503	83.905	181.357	1.00	110.84
25	4202	CA	ARG	D	440	64.231	84.774	182.276	1.00	110.52
	4203	CB	ARG	D	440	64.025	84.289	183.711	1.00	128.23
	4204	CG	ARG	D	440	62.627	83.749	184.002	1.00	153.84
	4205	CD	ARG	D	440	61.579	84.849	184.102	1.00	188.47
	4206	NE	ARG	D	440	60.232	84.332	183.856	1.00	215.81
30	4207	CZ	ARG	D	440	59.122	84.806	184.410	1.00	224.86
	4208	NH1	ARG	D	440	59.180	85.822	185.260	1.00	223.24
	4209	NH2	ARG	D	440	57.954	84.257	184.108	1.00	209.34
	4210	C	ARG	D	440	65.726	84.853	181.978	1.00	83.55
	4211	O	ARG	D	440	66.468	83.937	182.310	1.00	129.96
35	4212	N	ALA	D	441	66.172	85.951	181.372	1.00	74.53
	4213	CA	ALA	D	441	67.589	86.119	181.054	1.00	78.06
	4214	CB	ALA	D	441	67.753	86.473	179.593	1.00	98.44
	4215	C	ALA	D	441	68.222	87.195	181.922	1.00	73.89
	4216	O	ALA	D	441	67.781	88.340	181.908	1.00	87.18
40	4217	N	ALA	D	442	69.267	86.818	182.659	1.00	108.00
	4218	CA	ALA	D	442	69.993	87.722	183.560	1.00	84.59
	4219	CB	ALA	D	442	71.104	86.959	184.254	1.00	124.78
	4220	C	ALA	D	442	70.561	88.989	182.906	1.00	90.01
	4221	O	ALA	D	442	70.706	89.070	181.687	1.00	88.98
45	4222	N	PRO	D	443	70.904	89.993	183.725	1.00	81.16
	4223	CD	PRO	D	443	70.625	90.055	185.162	1.00	58.29
	4224	CA	PRO	D	443	71.449	91.273	183.272	1.00	65.44
	4225	CB	PRO	D	443	71.044	92.255	184.377	1.00	62.14
	4226	CG	PRO	D	443	70.143	91.467	185.294	1.00	84.05
50	4227	C	PRO	D	443	72.943	91.293	183.088	1.00	72.84
	4228	O	PRO	D	443	73.682	90.606	183.789	1.00	105.86
	4229	N	GLU	D	444	73.376	92.113	182.145	1.00	79.19
	4230	CA	GLU	D	444	74.782	92.292	181.855	1.00	104.43
	4231	CB	GLU	D	444	75.063	92.051	180.370	1.00	143.96
55	4232	CG	GLU	D	444	75.062	90.591	179.943	1.00	170.26

	4233	CD	GLU	D	444	74.905	90.425	178.443	1.00	152.52
	4234	OE1	GLU	D	444	75.481	91.243	177.693	1.00	116.93
	4235	OE2	GLU	D	444	74.210	89.475	178.018	1.00	138.72
	4236	C	GLU	D	444	74.992	93.747	182.180	1.00	84.83
5	4237	O	GLU	D	444	74.317	94.602	181.616	1.00	95.04
	4238	N	VAL	D	445	75.902	94.043	183.097	1.00	87.28
	4239	CA	VAL	D	445	76.152	95.433	183.453	1.00	76.03
	4240	CB	VAL	D	445	75.736	95.706	184.897	1.00	75.27
	4241	CG1	VAL	D	445	76.170	94.563	185.778	1.00	68.09
10	4242	CG2	VAL	D	445	76.333	97.020	185.366	1.00	93.41
	4243	C	VAL	D	445	77.599	95.863	183.264	1.00	60.53
	4244	O	VAL	D	445	78.520	95.096	183.545	1.00	92.85
	4245	N	TYR	D	446	77.791	97.090	182.783	1.00	65.90
	4246	CA	TYR	D	446	79.128	97.633	182.546	1.00	97.21
15	4247	CB	TYR	D	446	79.483	97.555	181.054	1.00	115.92
	4248	CG	TYR	D	446	79.187	96.214	180.416	1.00	124.25
	4249	CD1	TYR	D	446	78.088	96.048	179.579	1.00	108.68
	4250	CE1	TYR	D	446	77.774	94.803	179.036	1.00	143.50
	4251	CD2	TYR	D	446	79.975	95.097	180.692	1.00	175.81
20	4252	CE2	TYR	D	446	79.671	93.845	180.153	1.00	164.42
	4253	CZ	TYR	D	446	78.568	93.707	179.329	1.00	149.93
	4254	OH	TYR	D	446	78.246	92.473	178.813	1.00	162.97
	4255	C	TYR	D	446	79.143	99.086	182.995	1.00	97.06
	4256	O	TYR	D	446	78.386	99.896	182.470	1.00	99.04
25	4257	N	ALA	D	447	80.005	99.415	183.956	1.00	102.47
	4258	CA	ALA	D	447	80.100	100.782	184.484	1.00	66.24
	4259	CB	ALA	D	447	80.300	100.730	185.984	1.00	89.68
	4260	C	ALA	D	447	81.211	101.615	183.841	1.00	84.25
	4261	O	ALA	D	447	82.290	101.102	183.544	1.00	81.08
30	4262	N	PHE	D	448	80.957	102.906	183.642	1.00	53.71
	4263	CA	PHE	D	448	81.955	103.767	183.018	1.00	96.40
	4264	CB	PHE	D	448	81.528	104.081	181.583	1.00	110.89
	4265	CG	PHE	D	448	81.356	102.852	180.729	1.00	139.15
	4266	CD1	PHE	D	448	80.213	102.073	180.831	1.00	147.96
35	4267	CD2	PHE	D	448	82.368	102.438	179.872	1.00	185.33
	4268	CE1	PHE	D	448	80.080	100.901	180.100	1.00	149.26
	4269	CE2	PHE	D	448	82.246	101.267	179.135	1.00	184.09
	4270	CZ	PHE	D	448	81.099	100.497	179.250	1.00	182.71
	4271	C	PHE	D	448	82.240	105.047	183.799	1.00	83.02
40	4272	O	PHE	D	448	81.778	105.196	184.921	1.00	92.98
	4273	N	ALA	D	449	83.011	105.963	183.216	1.00	86.20
	4274	CA	ALA	D	449	83.363	107.210	183.901	1.00	46.82
	4275	CB	ALA	D	449	84.286	106.910	185.063	1.00	99.13
	4276	C	ALA	D	449	84.019	108.243	182.987	1.00	66.70
45	4277	O	ALA	D	449	85.007	107.964	182.302	1.00	82.28
	4278	N	THR	D	450	83.478	109.452	183.017	1.00	46.07
	4279	CA	THR	D	450	83.953	110.551	182.182	1.00	90.49
	4280	CB	THR	D	450	82.895	111.677	182.176	1.00	66.00
	4281	OG1	THR	D	450	81.684	111.176	181.611	1.00	102.05
50	4282	CG2	THR	D	450	83.355	112.870	181.373	1.00	103.25
	4283	C	THR	D	450	85.298	111.169	182.568	1.00	89.86
	4284	O	THR	D	450	85.722	111.083	183.711	1.00	116.46
	4285	N	PRO	D	451	86.004	111.760	181.590	1.00	87.34
	4286	CD	PRO	D	451	85.899	111.307	180.196	1.00	73.15
55	4287	CA	PRO	D	451	87.298	112.421	181.800	1.00	105.99

	4288	CB	PRO	D	451	87.997	112.253	180.450	1.00	127.70
	4289	CG	PRO	D	451	87.335	111.052	179.859	1.00	115.43
	4290	C	PRO	D	451	86.971	113.891	182.083	1.00	101.34
	4291	O	PRO	D	451	85.922	114.375	181.670	1.00	107.89
5	4292	N	GLU	D	452	87.850	114.611	182.768	1.00	115.89
	4293	CA	GLU	D	452	87.560	116.009	183.060	1.00	133.25
	4294	CB	GLU	D	452	88.700	116.645	183.863	1.00	159.83
	4295	CG	GLU	D	452	90.046	116.683	183.155	1.00	194.80
	4296	CD	GLU	D	452	91.097	117.446	183.947	1.00	196.79
10	4297	OE1	GLU	D	452	90.906	118.663	184.170	1.00	177.79
	4298	OE2	GLU	D	452	92.110	116.830	184.347	1.00	195.58
	4299	C	GLU	D	452	87.294	116.834	181.801	1.00	120.67
	4300	O	GLU	D	452	87.544	116.392	180.677	1.00	86.09
	4301	N	TRP	D	453	86.776	118.039	182.007	1.00	123.90
15	4302	CA	TRP	D	453	86.462	118.953	180.916	1.00	145.95
	4303	CB	TRP	D	453	84.992	118.777	180.504	1.00	170.02
	4304	CG	TRP	D	453	84.500	119.744	179.459	1.00	197.51
	4305	CD2	TRP	D	453	84.449	119.528	178.042	1.00	214.10
	4306	CE2	TRP	D	453	83.925	120.703	177.457	1.00	215.96
20	4307	CE3	TRP	D	453	84.792	118.453	177.210	1.00	219.72
	4308	CD1	TRP	D	453	84.022	121.006	179.668	1.00	209.18
	4309	NE1	TRP	D	453	83.675	121.589	178.471	1.00	210.81
	4310	CZ2	TRP	D	453	83.741	120.838	176.076	1.00	220.86
	4311	CZ3	TRP	D	453	84.609	118.587	175.834	1.00	220.01
25	4312	CH2	TRP	D	453	84.086	119.772	175.284	1.00	223.85
	4313	C	TRP	D	453	86.731	120.387	181.372	1.00	158.31
	4314	O	TRP	D	453	86.448	120.748	182.517	1.00	155.59
	4315	N	PRO	D	454	87.295	121.221	180.480	1.00	164.35
	4316	CD	PRO	D	454	87.673	120.851	179.102	1.00	146.83
30	4317	CA	PRO	D	454	87.624	122.628	180.746	1.00	184.14
	4318	CB	PRO	D	454	87.864	123.187	179.348	1.00	181.33
	4319	CG	PRO	D	454	88.523	122.033	178.664	1.00	173.35
	4320	C	PRO	D	454	86.558	123.418	181.509	1.00	195.45
	4321	O	PRO	D	454	86.855	124.447	182.116	1.00	210.90
35	4322	N	GLY	D	455	85.321	122.934	181.474	1.00	201.41
	4323	CA	GLY	D	455	84.239	123.613	182.165	1.00	189.27
	4324	C	GLY	D	455	84.373	123.555	183.674	1.00	182.16
	4325	O	GLY	D	455	84.142	124.550	184.362	1.00	191.75
	4326	N	SER	D	456	84.746	122.388	184.189	1.00	171.47
40	4327	CA	SER	D	456	84.913	122.193	185.625	1.00	166.50
	4328	CB	SER	D	456	83.591	121.774	186.261	1.00	158.47
	4329	OG	SER	D	456	83.188	120.511	185.764	1.00	140.37
	4330	C	SER	D	456	85.943	121.101	185.858	1.00	166.83
	4331	O	SER	D	456	85.996	120.122	185.114	1.00	174.49
45	4332	N	ARG	D	457	86.751	121.264	186.899	1.00	175.34
	4333	CA	ARG	D	457	87.787	120.288	187.213	1.00	178.26
	4334	CB	ARG	D	457	89.137	121.000	187.387	1.00	185.27
	4335	CG	ARG	D	457	89.546	121.846	186.184	1.00	203.14
	4336	CD	ARG	D	457	90.908	122.507	186.373	1.00	206.79
50	4337	NE	ARG	D	457	91.246	123.379	185.247	1.00	216.85
	4338	CZ	ARG	D	457	92.393	124.041	185.125	1.00	205.77
	4339	NH1	ARG	D	457	93.328	123.937	186.060	1.00	207.14
	4340	NH2	ARG	D	457	92.603	124.814	184.068	1.00	185.77
	4341	C	ARG	D	457	87.468	119.472	188.464	1.00	162.65
55	4342	O	ARG	D	457	88.291	118.675	188.915	1.00	168.22

	4343	N	ASP	D	458	86.274	119.660	189.018	1.00	149.08
	4344	CA	ASP	D	458	85.890	118.934	190.226	1.00	166.05
	4345	CB	ASP	D	458	85.908	119.875	191.434	1.00	188.82
	4346	CG	ASP	D	458	87.300	120.382	191.754	1.00	202.29
5	4347	OD1	ASP	D	458	88.212	119.544	191.919	1.00	202.70
	4348	OD2	ASP	D	458	87.480	121.615	191.843	1.00	197.86
	4349	C	ASP	D	458	84.531	118.249	190.137	1.00	167.63
	4350	O	ASP	D	458	83.930	117.904	191.158	1.00	106.20
	4351	N	LYS	D	459	84.055	118.053	188.912	1.00	184.87
10	4352	CA	LYS	D	459	82.773	117.395	188.672	1.00	167.70
	4353	CB	LYS	D	459	81.697	118.424	188.295	1.00	177.88
	4354	CG	LYS	D	459	81.395	119.467	189.373	1.00	201.66
	4355	CD	LYS	D	459	80.275	120.423	188.944	1.00	187.25
	4356	CE	LYS	D	459	79.958	121.446	190.038	1.00	173.49
15	4357	NZ	LYS	D	459	78.840	122.362	189.668	1.00	145.56
	4358	C	LYS	D	459	82.932	116.382	187.538	1.00	165.68
	4359	O	LYS	D	459	83.276	116.748	186.410	1.00	172.64
	4360	N	ARG	D	460	82.697	115.109	187.843	1.00	154.79
	4361	CA	ARG	D	460	82.804	114.051	186.841	1.00	153.22
20	4362	CB	ARG	D	460	84.095	113.244	187.058	1.00	125.90
	4363	CG	ARG	D	460	85.358	114.037	186.706	1.00	137.80
	4364	CD	ARG	D	460	86.588	113.151	186.537	1.00	147.84
	4365	NE	ARG	D	460	87.717	113.902	185.989	1.00	154.85
	4366	CZ	ARG	D	460	88.857	113.355	185.572	1.00	177.19
25	4367	NH1	ARG	D	460	89.037	112.042	185.634	1.00	158.76
	4368	NH2	ARG	D	460	89.824	114.124	185.090	1.00	193.89
	4369	C	ARG	D	460	81.561	113.141	186.828	1.00	141.33
	4370	O	ARG	D	460	81.033	112.758	187.876	1.00	118.12
	4371	N	THR	D	461	81.116	112.794	185.623	1.00	106.56
30	4372	CA	THR	D	461	79.912	111.998	185.408	1.00	72.86
	4373	CB	THR	D	461	79.214	112.496	184.135	1.00	85.08
	4374	OG1	THR	D	461	79.268	113.928	184.100	1.00	106.27
	4375	CG2	THR	D	461	77.771	112.026	184.092	1.00	59.78
	4376	C	THR	D	461	80.058	110.484	185.278	1.00	72.76
35	4377	O	THR	D	461	80.940	110.002	184.571	1.00	64.16
	4378	N	LEU	D	462	79.174	109.739	185.941	1.00	67.15
	4379	CA	LEU	D	462	79.176	108.269	185.838	1.00	93.90
	4380	CB	LEU	D	462	79.119	107.581	187.202	1.00	54.53
	4381	CG	LEU	D	462	80.338	107.682	188.115	1.00	86.30
40	4382	CD1	LEU	D	462	80.306	106.517	189.095	1.00	67.24
	4383	CD2	LEU	D	462	81.621	107.639	187.305	1.00	77.87
	4384	C	LEU	D	462	77.991	107.767	185.029	1.00	86.86
	4385	O	LEU	D	462	76.949	108.418	184.974	1.00	135.96
	4386	N	ALA	D	463	78.158	106.600	184.416	1.00	84.07
45	4387	CA	ALA	D	463	77.117	105.982	183.597	1.00	70.48
	4388	CB	ALA	D	463	77.311	106.345	182.132	1.00	69.52
	4389	C	ALA	D	463	77.176	104.476	183.773	1.00	66.61
	4390	O	ALA	D	463	78.250	103.897	183.916	1.00	72.40
	4391	N	CYS	D	464	76.021	103.837	183.750	1.00	69.61
50	4392	CA	CYS	D	464	75.980	102.407	183.946	1.00	72.19
	4393	C	CYS	D	464	74.947	101.799	183.022	1.00	95.42
	4394	O	CYS	D	464	73.769	102.144	183.080	1.00	118.74
	4395	CB	CYS	D	464	75.636	102.132	185.398	1.00	50.48
	4396	SG	CYS	D	464	75.624	100.393	185.919	1.00	118.72
55	4397	N	LEU	D	465	75.400	100.890	182.167	1.00	95.81

	4398	CA	LEU	D	465	74.530	100.233	181.207	1.00	80.91
	4399	CB	LEU	D	465	75.167	100.288	179.824	1.00	62.17
	4400	CG	LEU	D	465	74.700	99.281	178.772	1.00	81.47
	4401	CD1	LEU	D	465	73.187	99.193	178.728	1.00	87.06
5	4402	CD2	LEU	D	465	75.254	99.711	177.427	1.00	84.82
	4403	C	LEU	D	465	74.198	98.791	181.565	1.00	79.74
	4404	O	LEU	D	465	75.083	97.957	181.726	1.00	54.90
	4405	N	ILE	D	466	72.906	98.509	181.669	1.00	64.80
	4406	CA	ILE	D	466	72.437	97.182	182.007	1.00	58.32
10	4407	CB	ILE	D	466	71.567	97.232	183.254	1.00	77.30
	4408	CG2	ILE	D	466	71.276	95.823	183.747	1.00	58.46
	4409	CG1	ILE	D	466	72.281	98.066	184.316	1.00	44.32
	4410	CD1	ILE	D	466	71.633	98.043	185.670	1.00	83.41
	4411	C	ILE	D	466	71.624	96.670	180.837	1.00	93.77
15	4412	O	ILE	D	466	70.586	97.243	180.502	1.00	98.80
	4413	N	GLN	D	467	72.087	95.590	180.215	1.00	97.61
	4414	CA	GLN	D	467	71.385	95.063	179.060	1.00	69.11
	4415	CB	GLN	D	467	72.115	95.487	177.796	1.00	36.98
	4416	CG	GLN	D	467	73.590	95.168	177.789	1.00	80.17
20	4417	CD	GLN	D	467	74.224	95.357	176.419	1.00	115.95
	4418	OE1	GLN	D	467	74.035	96.388	175.759	1.00	80.89
	4419	NE2	GLN	D	467	74.989	94.359	175.986	1.00	133.96
	4420	C	GLN	D	467	71.124	93.570	178.994	1.00	43.59
	4421	O	GLN	D	467	71.414	92.816	179.917	1.00	51.62
25	4422	N	ASN	D	468	70.542	93.175	177.868	1.00	84.41
	4423	CA	ASN	D	468	70.204	91.797	177.562	1.00	78.87
	4424	CB	ASN	D	468	71.448	91.071	177.072	1.00	91.58
	4425	CG	ASN	D	468	72.167	91.847	175.992	1.00	131.22
	4426	OD1	ASN	D	468	71.557	92.267	175.000	1.00	109.30
30	4427	ND2	ASN	D	468	73.467	92.052	176.179	1.00	130.02
	4428	C	ASN	D	468	69.571	91.050	178.709	1.00	94.97
	4429	O	ASN	D	468	70.049	89.988	179.113	1.00	113.94
	4430	N	PHE	D	469	68.487	91.609	179.236	1.00	56.14
	4431	CA	PHE	D	469	67.783	90.960	180.327	1.00	70.60
35	4432	CB	PHE	D	469	68.001	91.710	181.643	1.00	43.17
	4433	CG	PHE	D	469	67.537	93.134	181.619	1.00	94.42
	4434	CD1	PHE	D	469	66.376	93.509	182.276	1.00	47.15
	4435	CD2	PHE	D	469	68.280	94.110	180.968	1.00	95.42
	4436	CE1	PHE	D	469	65.962	94.836	182.290	1.00	103.25
40	4437	CE2	PHE	D	469	67.877	95.441	180.978	1.00	28.33
	4438	CZ	PHE	D	469	66.716	95.804	181.639	1.00	101.58
	4439	C	PHE	D	469	66.308	90.888	180.020	1.00	67.94
	4440	O	PHE	D	469	65.834	91.535	179.083	1.00	51.85
	4441	N	MET	D	470	65.600	90.078	180.805	1.00	27.30
45	4442	CA	MET	D	470	64.158	89.910	180.673	1.00	69.57
	4443	CB	MET	D	470	63.814	89.320	179.308	1.00	108.06
	4444	CG	MET	D	470	64.665	88.140	178.901	1.00	121.33
	4445	SD	MET	D	470	64.817	88.077	177.103	1.00	132.64
	4446	CE	MET	D	470	63.162	87.566	176.645	1.00	170.43
50	4447	C	MET	D	470	63.637	89.020	181.785	1.00	73.39
	4448	O	MET	D	470	64.295	88.068	182.173	1.00	72.89
	4449	N	PRO	D	471	62.445	89.328	182.328	1.00	77.22
	4450	CD	PRO	D	471	61.921	88.464	183.393	1.00	79.25
	4451	CA	PRO	D	471	61.500	90.415	182.042	1.00	73.03
55	4452	CB	PRO	D	471	60.443	90.228	183.117	1.00	77.74

	4453	CG	PRO	D	471	60.456	88.748	183.334	1.00	95.61
	4454	C	PRO	D	471	62.108	91.805	182.094	1.00	66.54
	4455	O	PRO	D	471	63.298	91.962	182.323	1.00	79.62
	4456	N	GLU	D	472	61.280	92.819	181.886	1.00	87.24
	4457	CA	GLU	D	472	61.768	94.188	181.907	1.00	83.72
	4458	CB	GLU	D	472	60.933	95.063	180.969	1.00	104.73
	4459	CG	GLU	D	472	59.432	95.001	181.206	1.00	166.05
	4460	CD	GLU	D	472	58.686	96.116	180.490	1.00	187.22
	4461	OE1	GLU	D	472	58.879	96.275	179.267	1.00	172.24
	4462	OE2	GLU	D	472	57.904	96.834	181.149	1.00	193.81
	4463	C	GLU	D	472	61.770	94.796	183.304	1.00	104.32
	4464	O	GLU	D	472	62.261	95.906	183.487	1.00	102.37
	4465	N	ASP	D	473	61.233	94.077	184.288	1.00	59.56
	4466	CA	ASP	D	473	61.187	94.593	185.649	1.00	92.12
	4467	CB	ASP	D	473	60.234	93.756	186.504	1.00	116.46
	4468	CG	ASP	D	473	58.789	93.929	186.094	1.00	135.25
	4469	OD1	ASP	D	473	58.358	95.090	185.944	1.00	150.62
	4470	OD2	ASP	D	473	58.086	92.910	185.927	1.00	137.23
	4471	C	ASP	D	473	62.564	94.620	186.291	1.00	79.36
	4472	O	ASP	D	473	63.061	93.592	186.742	1.00	60.87
	4473	N	ILE	D	474	63.163	95.805	186.359	1.00	77.86
	4474	CA	ILE	D	474	64.493	95.947	186.935	1.00	57.62
	4475	CB	ILE	D	474	65.541	96.119	185.823	1.00	72.84
	4476	CG2	ILE	D	474	65.559	97.554	185.331	1.00	52.57
	4477	CG1	ILE	D	474	66.933	95.793	186.346	1.00	77.16
	4478	CD1	ILE	D	474	68.003	95.929	185.283	1.00	68.46
	4479	C	ILE	D	474	64.646	97.117	187.900	1.00	75.73
	4480	O	ILE	D	474	64.083	98.194	187.689	1.00	80.08
	4481	N	SER	D	475	65.427	96.893	188.952	1.00	67.18
	4482	CA	SER	D	475	65.698	97.914	189.957	1.00	72.99
	4483	CB	SER	D	475	65.258	97.429	191.351	1.00	63.48
	4484	OG	SER	D	475	63.999	97.964	191.727	1.00	93.55
	4485	C	SER	D	475	67.188	98.261	189.979	1.00	53.66
	4486	O	SER	D	475	68.017	97.470	190.419	1.00	75.03
	4487	N	VAL	D	476	67.521	99.448	189.499	1.00	55.61
	4488	CA	VAL	D	476	68.902	99.906	189.483	1.00	51.07
	4489	CB	VAL	D	476	69.166	100.775	188.240	1.00	63.18
	4490	CG1	VAL	D	476	70.539	101.424	188.313	1.00	61.47
	4491	CG2	VAL	D	476	69.062	99.927	187.005	1.00	79.72
	4492	C	VAL	D	476	69.166	100.749	190.728	1.00	58.51
	4493	O	VAL	D	476	68.232	101.248	191.346	1.00	116.08
	4494	N	GLN	D	477	70.436	100.908	191.085	1.00	70.31
	4495	CA	GLN	D	477	70.840	101.706	192.242	1.00	86.47
	4496	CB	GLN	D	477	70.317	101.076	193.526	1.00	59.72
	4497	CG	GLN	D	477	70.614	99.603	193.661	1.00	61.26
	4498	CD	GLN	D	477	69.958	99.013	194.889	1.00	111.88
	4499	OE1	GLN	D	477	68.738	99.086	195.044	1.00	120.03
	4500	NE2	GLN	D	477	70.761	98.429	195.775	1.00	97.73
	4501	C	GLN	D	477	72.355	101.845	192.331	1.00	83.04
	4502	O	GLN	D	477	73.095	101.333	191.489	1.00	85.92
	4503	N	TRP	D	478	72.829	102.546	193.349	1.00	78.76
	4504	CA	TRP	D	478	74.264	102.706	193.495	1.00	100.96
	4505	CB	TRP	D	478	74.714	104.068	192.967	1.00	36.74
	4506	CG	TRP	D	478	74.440	104.322	191.529	1.00	63.43
	4507	CD2	TRP	D	478	75.397	104.315	190.457	1.00	64.22

	4508	CE2	TRP	D	478	74.751	104.834	189.318	1.00	63.92
	4509	CE3	TRP	D	478	76.742	103.930	190.355	1.00	92.35
	4510	CD1	TRP	D	478	73.285	104.799	191.002	1.00	69.30
	4511	NE1	TRP	D	478	73.461	105.120	189.676	1.00	83.14
5	4512	CZ2	TRP	D	478	75.402	104.985	188.088	1.00	106.36
	4513	CZ3	TRP	D	478	77.391	104.080	189.132	1.00	74.82
	4514	CH2	TRP	D	478	76.719	104.606	188.016	1.00	79.83
	4515	C	TRP	D	478	74.723	102.569	194.938	1.00	79.39
	4516	O	TRP	D	478	73.959	102.797	195.866	1.00	116.11
10	4517	N	LEU	D	479	75.982	102.200	195.113	1.00	66.99
	4518	CA	LEU	D	479	76.560	102.055	196.428	1.00	70.32
	4519	CB	LEU	D	479	76.867	100.593	196.694	1.00	83.07
	4520	CG	LEU	D	479	75.686	99.688	196.347	1.00	60.88
	4521	CD1	LEU	D	479	76.079	98.229	196.566	1.00	143.46
15	4522	CD2	LEU	D	479	74.497	100.046	197.202	1.00	93.52
	4523	C	LEU	D	479	77.834	102.878	196.431	1.00	94.55
	4524	O	LEU	D	479	78.361	103.209	195.371	1.00	87.16
	4525	N	HIS	D	480	78.323	103.214	197.619	1.00	131.47
	4526	CA	HIS	D	480	79.537	104.013	197.746	1.00	117.34
20	4527	CB	HIS	D	480	79.249	105.474	197.383	1.00	110.78
	4528	CG	HIS	D	480	80.387	106.413	197.658	1.00	107.86
	4529	CD2	HIS	D	480	80.407	107.644	198.226	1.00	112.04
	4530	ND1	HIS	D	480	81.683	106.156	197.264	1.00	95.10
	4531	CE1	HIS	D	480	82.449	107.187	197.572	1.00	106.89
25	4532	NE2	HIS	D	480	81.698	108.104	198.156	1.00	113.38
	4533	C	HIS	D	480	80.068	103.931	199.157	1.00	92.28
	4534	O	HIS	D	480	79.612	104.647	200.049	1.00	92.69
	4535	N	ASN	D	481	81.028	103.043	199.362	1.00	97.73
	4536	CA	ASN	D	481	81.609	102.894	200.677	1.00	121.93
30	4537	CB	ASN	D	481	82.125	104.254	201.160	1.00	108.49
	4538	CG	ASN	D	481	83.258	104.126	202.145	1.00	147.00
	4539	OD1	ASN	D	481	83.876	105.120	202.522	1.00	154.08
	4540	ND2	ASN	D	481	83.542	102.897	202.570	1.00	166.29
	4541	C	ASN	D	481	80.546	102.355	201.630	1.00	81.70
35	4542	O	ASN	D	481	80.382	102.854	202.746	1.00	102.35
	4543	N	GLU	D	482	79.817	101.342	201.169	1.00	78.94
	4544	CA	GLU	D	482	78.776	100.706	201.975	1.00	126.14
	4545	CB	GLU	D	482	79.365	100.258	203.324	1.00	135.98
	4546	CG	GLU	D	482	80.643	99.421	203.217	1.00	152.58
40	4547	CD	GLU	D	482	80.427	98.088	202.517	1.00	174.16
	4548	OE1	GLU	D	482	79.638	97.265	203.030	1.00	170.45
	4549	OE2	GLU	D	482	81.047	97.863	201.455	1.00	174.56
	4550	C	GLU	D	482	77.575	101.627	202.215	1.00	109.93
	4551	O	GLU	D	482	76.820	101.447	203.175	1.00	82.30
45	4552	N	VAL	D	483	77.392	102.605	201.336	1.00	76.74
	4553	CA	VAL	D	483	76.287	103.551	201.477	1.00	102.62
	4554	CB	VAL	D	483	76.815	104.983	201.744	1.00	109.65
	4555	CG1	VAL	D	483	75.669	105.986	201.713	1.00	98.68
	4556	CG2	VAL	D	483	77.519	105.028	203.088	1.00	170.08
50	4557	C	VAL	D	483	75.392	103.588	200.243	1.00	117.05
	4558	O	VAL	D	483	75.779	104.119	199.202	1.00	143.84
	4559	N	GLN	D	484	74.193	103.027	200.365	1.00	104.30
	4560	CA	GLN	D	484	73.244	103.003	199.258	1.00	63.80
	4561	CB	GLN	D	484	72.062	102.112	199.617	1.00	106.13
55	4562	CG	GLN	D	484	71.037	101.964	198.510	1.00	90.87

	4563	CD	GLN	D	484	69.823	101.181	198.969	1.00	129.10
	4564	OE1	GLN	D	484	69.946	100.156	199.659	1.00	95.62
	4565	NE2	GLN	D	484	68.639	101.654	198.587	1.00	134.96
	4566	C	GLN	D	484	72.750	104.413	198.969	1.00	52.20
5	4567	O	GLN	D	484	71.799	104.874	199.588	1.00	109.44
	4568	N	LEU	D	485	73.377	105.098	198.024	1.00	55.15
	4569	CA	LEU	D	485	72.991	106.471	197.711	1.00	71.69
	4570	CB	LEU	D	485	73.698	106.961	196.447	1.00	66.01
	4571	CG	LEU	D	485	75.216	107.146	196.541	1.00	75.22
10	4572	CD1	LEU	D	485	75.661	108.084	195.431	1.00	81.39
	4573	CD2	LEU	D	485	75.604	107.739	197.885	1.00	111.54
	4574	C	LEU	D	485	71.504	106.758	197.579	1.00	78.22
	4575	O	LEU	D	485	70.698	105.854	197.350	1.00	76.73
	4576	N	PRO	D	486	71.127	108.040	197.735	1.00	77.50
15	4577	CD	PRO	D	486	72.025	109.127	198.161	1.00	119.22
	4578	CA	PRO	D	486	69.749	108.532	197.646	1.00	96.61
	4579	CB	PRO	D	486	69.876	110.004	198.038	1.00	131.87
	4580	CG	PRO	D	486	71.086	110.026	198.916	1.00	136.66
	4581	C	PRO	D	486	69.179	108.380	196.244	1.00	92.91
20	4582	O	PRO	D	486	69.756	108.858	195.264	1.00	55.14
	4583	N	ASP	D	487	68.027	107.731	196.163	1.00	82.83
	4584	CA	ASP	D	487	67.380	107.504	194.888	1.00	93.17
	4585	CB	ASP	D	487	65.947	107.016	195.124	1.00	115.19
	4586	CG	ASP	D	487	65.437	106.130	193.996	1.00	161.24
25	4587	OD1	ASP	D	487	65.248	106.640	192.869	1.00	164.95
	4588	OD2	ASP	D	487	65.232	104.918	194.235	1.00	171.27
	4589	C	ASP	D	487	67.383	108.752	193.995	1.00	74.98
	4590	O	ASP	D	487	67.617	108.660	192.791	1.00	95.57
	4591	N	ALA	D	488	67.149	109.920	194.583	1.00	74.62
30	4592	CA	ALA	D	488	67.100	111.162	193.812	1.00	77.13
	4593	CB	ALA	D	488	66.474	112.268	194.656	1.00	113.89
	4594	C	ALA	D	488	68.455	111.622	193.277	1.00	89.67
	4595	O	ALA	D	488	68.559	112.683	192.647	1.00	78.05
	4596	N	ARG	D	489	69.489	110.822	193.520	1.00	47.18
35	4597	CA	ARG	D	489	70.837	111.159	193.065	1.00	81.70
	4598	CB	ARG	D	489	71.856	110.474	193.974	1.00	98.18
	4599	CG	ARG	D	489	72.159	111.254	195.231	1.00	119.10
	4600	CD	ARG	D	489	73.301	112.214	194.975	1.00	108.85
	4601	NE	ARG	D	489	74.572	111.660	195.432	1.00	107.43
40	4602	CZ	ARG	D	489	75.764	112.102	195.042	1.00	115.63
	4603	NH1	ARG	D	489	75.858	113.107	194.175	1.00	102.89
	4604	NH2	ARG	D	489	76.863	111.548	195.532	1.00	113.00
	4605	C	ARG	D	489	71.146	110.806	191.606	1.00	93.41
	4606	O	ARG	D	489	71.879	111.526	190.920	1.00	91.06
45	4607	N	HIS	D	490	70.579	109.699	191.138	1.00	91.66
	4608	CA	HIS	D	490	70.810	109.230	189.784	1.00	79.10
	4609	CB	HIS	D	490	71.330	107.809	189.831	1.00	61.88
	4610	CG	HIS	D	490	70.361	106.847	190.429	1.00	50.09
	4611	CD2	HIS	D	490	69.154	106.414	189.998	1.00	71.95
50	4612	ND1	HIS	D	490	70.600	106.198	191.622	1.00	80.99
	4613	CE1	HIS	D	490	69.582	105.403	191.899	1.00	81.13
	4614	NE2	HIS	D	490	68.691	105.516	190.929	1.00	120.64
	4615	C	HIS	D	490	69.567	109.238	188.925	1.00	73.38
	4616	O	HIS	D	490	68.455	109.193	189.431	1.00	83.57
55	4617	N	SER	D	491	69.773	109.267	187.616	1.00	106.32

	4618	CA	SER	D	491	68.676	109.246	186.663	1.00	99.85
	4619	CB	SER	D	491	68.783	110.424	185.696	1.00	80.79
	4620	OG	SER	D	491	67.681	110.437	184.802	1.00	153.32
	4621	C	SER	D	491	68.731	107.937	185.879	1.00	95.44
5	4622	O	SER	D	491	69.712	107.647	185.204	1.00	77.44
	4623	N	THR	D	492	67.678	107.140	185.974	1.00	107.33
	4624	CA	THR	D	492	67.638	105.879	185.254	1.00	88.96
	4625	CB	THR	D	492	67.385	104.714	186.217	1.00	93.46
	4626	OG1	THR	D	492	68.540	104.532	187.044	1.00	95.38
10	4627	CG2	THR	D	492	67.093	103.435	185.453	1.00	86.11
	4628	C	THR	D	492	66.529	105.932	184.216	1.00	97.57
	4629	O	THR	D	492	65.418	106.361	184.520	1.00	115.51
	4630	N	THR	D	493	66.826	105.501	182.993	1.00	66.72
	4631	CA	THR	D	493	65.820	105.527	181.936	1.00	75.38
15	4632	CB	THR	D	493	66.444	105.482	180.543	1.00	81.55
	4633	OG1	THR	D	493	66.925	104.157	180.285	1.00	66.75
	4634	CG2	THR	D	493	67.587	106.470	180.445	1.00	83.27
	4635	C	THR	D	493	64.856	104.354	182.017	1.00	88.44
	4636	O	THR	D	493	64.911	103.529	182.941	1.00	70.82
20	4637	N	GLN	D	494	63.964	104.296	181.036	1.00	95.57
	4638	CA	GLN	D	494	62.988	103.229	180.976	1.00	86.74
	4639	CB	GLN	D	494	61.641	103.773	180.491	1.00	104.79
	4640	CG	GLN	D	494	61.002	104.821	181.399	1.00	121.61
	4641	CD	GLN	D	494	60.761	104.317	182.821	1.00	154.81
25	4642	OE1	GLN	D	494	60.297	103.194	183.027	1.00	127.19
	4643	NE2	GLN	D	494	61.064	105.158	183.806	1.00	163.95
	4644	C	GLN	D	494	63.500	102.163	180.014	1.00	105.68
	4645	O	GLN	D	494	64.174	102.473	179.029	1.00	117.51
	4646	N	PRO	D	495	63.204	100.889	180.301	1.00	74.85
30	4647	CD	PRO	D	495	62.540	100.401	181.518	1.00	68.14
	4648	CA	PRO	D	495	63.620	99.765	179.469	1.00	67.40
	4649	CB	PRO	D	495	62.844	98.607	180.069	1.00	57.90
	4650	CG	PRO	D	495	62.886	98.927	181.501	1.00	51.00
	4651	C	PRO	D	495	63.295	99.968	177.996	1.00	77.06
35	4652	O	PRO	D	495	62.317	100.621	177.647	1.00	102.71
	4653	N	ARG	D	496	64.136	99.410	177.138	1.00	110.77
	4654	CA	ARG	D	496	63.956	99.496	175.697	1.00	122.60
	4655	CB	ARG	D	496	64.765	100.668	175.128	1.00	143.51
	4656	CG	ARG	D	496	64.080	102.027	175.280	1.00	154.62
40	4657	CD	ARG	D	496	65.003	103.174	174.882	1.00	172.80
	4658	NE	ARG	D	496	64.275	104.427	174.686	1.00	206.30
	4659	CZ	ARG	D	496	63.560	104.716	173.603	1.00	204.90
	4660	NH1	ARG	D	496	63.477	103.842	172.608	1.00	198.29
	4661	NH2	ARG	D	496	62.923	105.877	173.515	1.00	192.83
45	4662	C	ARG	D	496	64.426	98.170	175.119	1.00	131.58
	4663	O	ARG	D	496	65.365	97.568	175.630	1.00	107.54
	4664	N	LYS	D	497	63.767	97.707	174.063	1.00	139.06
	4665	CA	LYS	D	497	64.114	96.427	173.459	1.00	98.97
	4666	CB	LYS	D	497	62.936	95.900	172.636	1.00	111.63
50	4667	CG	LYS	D	497	61.645	95.750	173.428	1.00	148.53
	4668	CD	LYS	D	497	60.515	95.187	172.575	1.00	162.48
	4669	CE	LYS	D	497	59.221	95.078	173.374	1.00	159.87
	4670	NZ	LYS	D	497	58.111	94.478	172.579	1.00	147.14
	4671	C	LYS	D	497	65.360	96.466	172.594	1.00	102.21
55	4672	O	LYS	D	497	65.804	97.525	172.155	1.00	87.29

	4673	N	THR	D	498	65.919	95.287	172.358	1.00	121.14
	4674	CA	THR	D	498	67.108	95.144	171.536	1.00	136.22
	4675	CB	THR	D	498	68.350	94.851	172.400	1.00	124.43
	4676	OG1	THR	D	498	68.079	93.769	173.302	1.00	102.03
	4677	CG2	THR	D	498	68.724	96.073	173.194	1.00	135.22
	4678	C	THR	D	498	66.928	94.020	170.520	1.00	160.20
	4679	O	THR	D	498	66.064	93.148	170.677	1.00	127.05
	4680	N	LYS	D	499	67.746	94.045	169.473	1.00	148.81
	4681	CA	LYS	D	499	67.665	93.030	168.436	1.00	167.95
	4682	CB	LYS	D	499	68.518	93.442	167.227	1.00	183.82
	4683	CG	LYS	D	499	68.240	92.635	165.953	1.00	194.67
	4684	CD	LYS	D	499	68.915	93.247	164.723	1.00	178.66
	4685	CE	LYS	D	499	68.530	92.509	163.439	1.00	166.21
	4686	NZ	LYS	D	499	69.080	93.166	162.212	1.00	129.82
	4687	C	LYS	D	499	68.131	91.685	168.993	1.00	174.78
	4688	O	LYS	D	499	68.477	90.773	168.243	1.00	193.59
	4689	N	GLY	D	500	68.132	91.570	170.318	1.00	172.34
	4690	CA	GLY	D	500	68.549	90.339	170.963	1.00	167.96
	4691	C	GLY	D	500	67.489	89.841	171.925	1.00	174.62
	4692	O	GLY	D	500	67.796	89.121	172.875	1.00	180.27
	4693	N	SER	D	501	66.244	90.244	171.674	1.00	149.85
	4694	CA	SER	D	501	65.086	89.863	172.485	1.00	145.87
	4695	CB	SER	D	501	64.828	88.355	172.379	1.00	150.97
	4696	OG	SER	D	501	65.865	87.601	172.983	1.00	182.29
	4697	C	SER	D	501	65.171	90.255	173.960	1.00	148.85
	4698	O	SER	D	501	64.317	89.871	174.758	1.00	131.95
	4699	N	GLY	D	502	66.194	91.018	174.322	1.00	141.68
	4700	CA	GLY	D	502	66.334	91.439	175.703	1.00	99.20
	4701	C	GLY	D	502	66.210	92.943	175.805	1.00	120.83
	4702	O	GLY	D	502	66.192	93.629	174.781	1.00	107.61
	4703	N	PHE	D	503	66.121	93.465	177.027	1.00	106.97
	4704	CA	PHE	D	503	66.005	94.906	177.208	1.00	87.81
	4705	CB	PHE	D	503	64.911	95.253	178.201	1.00	59.57
	4706	CG	PHE	D	503	63.595	94.625	177.908	1.00	73.29
	4707	CD1	PHE	D	503	63.264	93.397	178.453	1.00	86.43
	4708	CD2	PHE	D	503	62.658	95.290	177.144	1.00	53.84
	4709	CE1	PHE	D	503	62.015	92.845	178.250	1.00	84.48
	4710	CE2	PHE	D	503	61.404	94.747	176.932	1.00	115.27
	4711	CZ	PHE	D	503	61.081	93.520	177.490	1.00	109.78
	4712	C	PHE	D	503	67.293	95.543	177.700	1.00	86.70
	4713	O	PHE	D	503	68.236	94.851	178.074	1.00	68.11
	4714	N	PHE	D	504	67.304	96.874	177.720	1.00	64.93
	4715	CA	PHE	D	504	68.463	97.628	178.160	1.00	58.80
	4716	CB	PHE	D	504	69.399	97.867	176.972	1.00	62.27
	4717	CG	PHE	D	504	69.039	99.068	176.119	1.00	49.02
	4718	CD1	PHE	D	504	69.470	100.338	176.467	1.00	69.40
	4719	CD2	PHE	D	504	68.314	98.916	174.948	1.00	92.30
	4720	CE1	PHE	D	504	69.192	101.431	175.665	1.00	83.85
	4721	CE2	PHE	D	504	68.030	100.006	174.138	1.00	117.28
	4722	CZ	PHE	D	504	68.474	101.266	174.498	1.00	115.08
	4723	C	PHE	D	504	68.066	98.962	178.779	1.00	67.09
	4724	O	PHE	D	504	67.236	99.690	178.233	1.00	100.63
	4725	N	VAL	D	505	68.662	99.283	179.920	1.00	82.59
	4726	CA	VAL	D	505	68.376	100.546	180.583	1.00	86.93
	4727	CB	VAL	D	505	67.554	100.339	181.865	1.00	66.93

	4728	CG1	VAL	D	505	68.374	99.626	182.909	1.00	44.42
	4729	CG2	VAL	D	505	67.089	101.683	182.388	1.00	110.77
	4730	C	VAL	D	505	69.672	101.266	180.936	1.00	63.33
	4731	O	VAL	D	505	70.685	100.634	181.212	1.00	81.80
5	4732	N	PHE	D	506	69.629	102.592	180.924	1.00	82.05
	4733	CA	PHE	D	506	70.796	103.414	181.227	1.00	74.33
	4734	CB	PHE	D	506	71.026	104.405	180.096	1.00	64.40
	4735	CG	PHE	D	506	71.958	103.925	179.028	1.00	65.82
	4736	CD1	PHE	D	506	71.821	104.396	177.728	1.00	93.15
10	4737	CD2	PHE	D	506	73.015	103.082	179.321	1.00	97.38
	4738	CE1	PHE	D	506	72.715	104.046	176.741	1.00	60.40
	4739	CE2	PHE	D	506	73.920	102.723	178.335	1.00	94.39
	4740	CZ	PHE	D	506	73.770	103.207	177.044	1.00	83.28
	4741	C	PHE	D	506	70.632	104.203	182.525	1.00	84.85
15	4742	O	PHE	D	506	69.530	104.648	182.857	1.00	134.54
	4743	N	SER	D	507	71.736	104.387	183.248	1.00	93.21
	4744	CA	SER	D	507	71.722	105.144	184.500	1.00	85.59
	4745	CB	SER	D	507	71.894	104.219	185.700	1.00	41.54
	4746	OG	SER	D	507	71.868	104.985	186.887	1.00	68.49
20	4747	C	SER	D	507	72.833	106.187	184.516	1.00	67.47
	4748	O	SER	D	507	73.925	105.945	184.012	1.00	59.51
	4749	N	ARG	D	508	72.550	107.342	185.105	1.00	61.04
	4750	CA	ARG	D	508	73.517	108.428	185.175	1.00	58.84
	4751	CB	ARG	D	508	73.139	109.517	184.167	1.00	49.25
25	4752	CG	ARG	D	508	73.977	110.781	184.239	1.00	60.80
	4753	CD	ARG	D	508	73.595	111.707	183.087	1.00	74.40
	4754	NE	ARG	D	508	74.244	113.013	183.150	1.00	57.97
	4755	CZ	ARG	D	508	73.940	113.952	184.042	1.00	108.28
	4756	NH1	ARG	D	508	72.994	113.730	184.947	1.00	134.73
30	4757	NH2	ARG	D	508	74.574	115.118	184.028	1.00	134.59
	4758	C	ARG	D	508	73.579	108.999	186.586	1.00	66.73
	4759	O	ARG	D	508	72.559	109.381	187.162	1.00	94.10
	4760	N	LEU	D	509	74.792	109.076	187.123	1.00	102.57
	4761	CA	LEU	D	509	75.009	109.556	188.479	1.00	92.49
35	4762	CB	LEU	D	509	75.349	108.353	189.361	1.00	65.32
	4763	CG	LEU	D	509	75.820	108.672	190.775	1.00	82.75
	4764	CD1	LEU	D	509	74.814	109.609	191.434	1.00	121.62
	4765	CD2	LEU	D	509	75.980	107.383	191.571	1.00	45.98
	4766	C	LEU	D	509	76.108	110.609	188.620	1.00	66.30
40	4767	O	LEU	D	509	77.252	110.253	188.843	1.00	62.93
	4768	N	GLU	D	510	75.774	111.893	188.504	1.00	101.58
	4769	CA	GLU	D	510	76.793	112.943	188.641	1.00	93.28
	4770	CB	GLU	D	510	76.143	114.333	188.575	1.00	108.16
	4771	CG	GLU	D	510	75.472	114.649	187.240	1.00	127.89
45	4772	CD	GLU	D	510	74.727	115.982	187.233	1.00	158.27
	4773	OE1	GLU	D	510	73.731	116.114	187.978	1.00	163.67
	4774	OE2	GLU	D	510	75.133	116.898	186.481	1.00	133.07
	4775	C	GLU	D	510	77.516	112.757	189.981	1.00	107.52
	4776	O	GLU	D	510	76.906	112.303	190.949	1.00	106.06
50	4777	N	VAL	D	511	78.808	113.095	190.036	1.00	92.80
	4778	CA	VAL	D	511	79.599	112.937	191.268	1.00	119.85
	4779	CB	VAL	D	511	80.495	111.658	191.193	1.00	42.93
	4780	CG1	VAL	D	511	81.422	111.579	192.387	1.00	117.40
	4781	CG2	VAL	D	511	79.622	110.425	191.171	1.00	107.86
55	4782	C	VAL	D	511	80.483	114.145	191.640	1.00	159.37

	4783	O	VAL	D	511	80.869	114.943	190.776	1.00	157.18
	4784	N	THR	D	512	80.795	114.261	192.936	1.00	172.76
	4785	CA	THR	D	512	81.622	115.346	193.472	1.00	158.22
	4786	CB	THR	D	512	80.946	116.001	194.700	1.00	168.13
5	4787	OG1	THR	D	512	79.636	116.460	194.340	1.00	167.64
	4788	CG2	THR	D	512	81.773	117.182	195.203	1.00	185.75
	4789	C	THR	D	512	83.020	114.866	193.889	1.00	141.73
	4790	O	THR	D	512	83.171	113.781	194.468	1.00	95.92
	4791	N	ARG	D	513	84.029	115.691	193.598	1.00	133.96
10	4792	CA	ARG	D	513	85.423	115.383	193.919	1.00	137.46
	4793	CB	ARG	D	513	86.296	116.640	193.794	1.00	162.09
	4794	CG	ARG	D	513	87.780	116.393	194.082	1.00	185.62
	4795	CD	ARG	D	513	88.601	117.679	194.049	1.00	208.34
	4796	NE	ARG	D	513	90.013	117.433	194.340	1.00	232.40
15	4797	CZ	ARG	D	513	90.943	118.383	194.427	1.00	235.91
	4798	NH1	ARG	D	513	90.620	119.656	194.244	1.00	230.77
	4799	NH2	ARG	D	513	92.201	118.059	194.699	1.00	224.77
	4800	C	ARG	D	513	85.580	114.803	195.315	1.00	122.87
	4801	O	ARG	D	513	86.170	113.737	195.499	1.00	77.13
20	4802	N	ALA	D	514	85.050	115.520	196.295	1.00	123.66
	4803	CA	ALA	D	514	85.120	115.095	197.682	1.00	119.89
	4804	CB	ALA	D	514	84.105	115.872	198.496	1.00	121.33
	4805	C	ALA	D	514	84.881	113.594	197.847	1.00	114.46
	4806	O	ALA	D	514	85.618	112.909	198.559	1.00	115.15
25	4807	N	GLU	D	515	83.860	113.086	197.165	1.00	114.63
	4808	CA	GLU	D	515	83.502	111.677	197.265	1.00	110.01
	4809	CB	GLU	D	515	82.120	111.454	196.648	1.00	77.08
	4810	CG	GLU	D	515	81.013	112.106	197.450	1.00	144.14
	4811	CD	GLU	D	515	79.656	111.961	196.806	1.00	162.03
30	4812	OE1	GLU	D	515	79.475	112.477	195.680	1.00	133.35
	4813	OE2	GLU	D	515	78.773	111.334	197.431	1.00	167.09
	4814	C	GLU	D	515	84.480	110.641	196.718	1.00	110.50
	4815	O	GLU	D	515	84.593	109.548	197.282	1.00	87.75
	4816	N	TRP	D	516	85.188	110.948	195.635	1.00	88.87
35	4817	CA	TRP	D	516	86.111	109.943	195.117	1.00	96.30
	4818	CB	TRP	D	516	86.285	110.065	193.596	1.00	116.50
	4819	CG	TRP	D	516	87.195	111.132	193.088	1.00	89.33
	4820	CD2	TRP	D	516	86.815	112.276	192.315	1.00	84.44
	4821	CE2	TRP	D	516	88.002	112.945	191.949	1.00	97.81
40	4822	CE3	TRP	D	516	85.585	112.796	191.892	1.00	94.14
	4823	CD1	TRP	D	516	88.556	111.159	193.168	1.00	124.94
	4824	NE1	TRP	D	516	89.050	112.243	192.483	1.00	140.17
	4825	CZ2	TRP	D	516	87.996	114.115	191.178	1.00	128.17
	4826	CZ3	TRP	D	516	85.578	113.960	191.125	1.00	81.83
45	4827	CH2	TRP	D	516	86.779	114.604	190.775	1.00	116.38
	4828	C	TRP	D	516	87.452	109.954	195.824	1.00	127.96
	4829	O	TRP	D	516	88.268	109.049	195.640	1.00	148.49
	4830	N	GLU	D	517	87.676	110.982	196.636	1.00	129.08
	4831	CA	GLU	D	517	88.906	111.068	197.400	1.00	111.06
50	4832	CB	GLU	D	517	89.239	112.523	197.722	1.00	135.30
	4833	CG	GLU	D	517	89.577	113.349	196.490	1.00	155.78
	4834	CD	GLU	D	517	90.194	114.688	196.834	1.00	196.31
	4835	OE1	GLU	D	517	89.548	115.475	197.559	1.00	211.98
	4836	OE2	GLU	D	517	91.328	114.952	196.380	1.00	180.61
55	4837	C	GLU	D	517	88.632	110.271	198.668	1.00	124.76

	4838	O	GLU	D	517	89.549	109.710	199.278	1.00	141.89
	4839	N	GLN	D	518	87.352	110.217	199.041	1.00	103.46
	4840	CA	GLN	D	518	86.906	109.467	200.211	1.00	115.30
	4841	CB	GLN	D	518	85.419	109.731	200.463	1.00	143.81
5	4842	CG	GLN	D	518	84.866	109.115	201.744	1.00	176.95
	4843	CD	GLN	D	518	83.365	109.327	201.897	1.00	168.05
	4844	OE1	GLN	D	518	82.879	110.461	201.875	1.00	121.65
	4845	NE2	GLN	D	518	82.624	108.233	202.053	1.00	146.22
	4846	C	GLN	D	518	87.136	107.988	199.890	1.00	126.60
10	4847	O	GLN	D	518	87.433	107.182	200.778	1.00	97.98
	4848	N	LYS	D	519	86.987	107.660	198.605	1.00	133.48
	4849	CA	LYS	D	519	87.195	106.314	198.065	1.00	130.66
	4850	CB	LYS	D	519	86.243	105.295	198.698	1.00	75.97
	4851	CG	LYS	D	519	86.644	103.852	198.402	1.00	89.89
15	4852	CD	LYS	D	519	86.097	102.873	199.431	1.00	118.90
	4853	CE	LYS	D	519	86.781	101.513	199.312	1.00	120.25
	4854	NZ	LYS	D	519	86.331	100.555	200.365	1.00	142.07
	4855	C	LYS	D	519	86.960	106.353	196.560	1.00	122.50
	4856	O	LYS	D	519	86.313	107.271	196.063	1.00	112.56
20	4857	N	ASP	D	520	87.494	105.364	195.840	1.00	147.72
	4858	CA	ASP	D	520	87.334	105.277	194.383	1.00	101.05
	4859	CB	ASP	D	520	88.642	104.843	193.718	1.00	139.44
	4860	CG	ASP	D	520	89.593	105.997	193.499	1.00	177.33
	4861	OD1	ASP	D	520	89.228	106.917	192.737	1.00	157.39
25	4862	OD2	ASP	D	520	90.698	105.982	194.086	1.00	181.89
	4863	C	ASP	D	520	86.240	104.292	193.999	1.00	90.40
	4864	O	ASP	D	520	85.540	104.494	193.015	1.00	100.30
	4865	N	GLU	D	521	86.104	103.225	194.783	1.00	113.97
	4866	CA	GLU	D	521	85.096	102.196	194.535	1.00	100.63
30	4867	CB	GLU	D	521	85.165	101.093	195.599	1.00	137.88
	4868	CG	GLU	D	521	85.922	99.836	195.206	1.00	152.59
	4869	CD	GLU	D	521	85.646	98.680	196.162	1.00	162.69
	4870	OE1	GLU	D	521	84.480	98.228	196.228	1.00	124.80
	4871	OE2	GLU	D	521	86.587	98.228	196.850	1.00	167.89
35	4872	C	GLU	D	521	83.661	102.715	194.504	1.00	98.08
	4873	O	GLU	D	521	83.099	103.086	195.534	1.00	104.25
	4874	N	PHE	D	522	83.078	102.726	193.312	1.00	127.92
	4875	CA	PHE	D	522	81.692	103.137	193.112	1.00	85.49
	4876	CB	PHE	D	522	81.596	104.278	192.104	1.00	55.87
40	4877	CG	PHE	D	522	81.809	105.627	192.700	1.00	92.01
	4878	CD1	PHE	D	522	82.876	105.862	193.553	1.00	109.83
	4879	CD2	PHE	D	522	80.950	106.672	192.392	1.00	125.42
	4880	CE1	PHE	D	522	83.080	107.123	194.087	1.00	147.56
	4881	CE2	PHE	D	522	81.146	107.935	192.919	1.00	81.53
45	4882	CZ	PHE	D	522	82.208	108.163	193.765	1.00	99.48
	4883	C	PHE	D	522	80.989	101.915	192.556	1.00	91.67
	4884	O	PHE	D	522	81.450	101.315	191.587	1.00	86.92
	4885	N	ILE	D	523	79.879	101.532	193.159	1.00	58.82
	4886	CA	ILE	D	523	79.199	100.360	192.670	1.00	96.62
50	4887	CB	ILE	D	523	79.059	99.315	193.791	1.00	67.53
	4888	CG2	ILE	D	523	78.386	98.043	193.261	1.00	71.95
	4889	CG1	ILE	D	523	80.448	98.994	194.353	1.00	74.60
	4890	CD1	ILE	D	523	80.448	97.914	195.426	1.00	142.45
	4891	C	ILE	D	523	77.839	100.700	192.098	1.00	86.74
55	4892	O	ILE	D	523	77.110	101.506	192.654	1.00	100.77

	4893	N	CYS	D	524	77.521	100.095	190.961	1.00	98.48
	4894	CA	CYS	D	524	76.236	100.283	190.304	1.00	85.44
	4895	C	CYS	D	524	75.553	98.922	190.326	1.00	64.47
	4896	O	CYS	D	524	75.712	98.128	189.406	1.00	68.44
	4897	CB	CYS	D	524	76.425	100.739	188.861	1.00	71.53
	4898	SG	CYS	D	524	74.938	100.516	187.836	1.00	110.38
	4899	N	ARG	D	525	74.809	98.655	191.395	1.00	92.59
	4900	CA	ARG	D	525	74.107	97.387	191.569	1.00	59.38
	4901	CB	ARG	D	525	73.679	97.234	193.029	1.00	53.65
	4902	CG	ARG	D	525	73.283	95.825	193.416	1.00	62.42
	4903	CD	ARG	D	525	73.547	95.533	194.901	1.00	81.91
	4904	NE	ARG	D	525	72.599	96.177	195.808	1.00	90.24
	4905	CZ	ARG	D	525	72.458	95.846	197.088	1.00	147.65
	4906	NH1	ARG	D	525	73.206	94.878	197.608	1.00	136.10
	4907	NH2	ARG	D	525	71.568	96.475	197.847	1.00	130.51
	4908	C	ARG	D	525	72.890	97.286	190.665	1.00	81.55
	4909	O	ARG	D	525	72.477	98.264	190.048	1.00	81.39
	4910	N	ALA	D	526	72.325	96.089	190.590	1.00	78.78
	4911	CA	ALA	D	526	71.152	95.837	189.770	1.00	57.14
	4912	CB	ALA	D	526	71.564	95.534	188.356	1.00	39.11
	4913	C	ALA	D	526	70.393	94.661	190.359	1.00	60.25
	4914	O	ALA	D	526	70.982	93.665	190.776	1.00	67.91
	4915	N	VAL	D	527	69.078	94.783	190.403	1.00	45.78
	4916	CA	VAL	D	527	68.265	93.721	190.958	1.00	62.42
	4917	CB	VAL	D	527	67.445	94.234	192.147	1.00	81.54
	4918	CG1	VAL	D	527	66.648	93.095	192.766	1.00	72.43
	4919	CG2	VAL	D	527	68.373	94.871	193.163	1.00	71.57
	4920	C	VAL	D	527	67.326	93.199	189.894	1.00	54.64
	4921	O	VAL	D	527	66.520	93.949	189.356	1.00	97.00
	4922	N	HIS	D	528	67.443	91.914	189.584	1.00	64.63
	4923	CA	HIS	D	528	66.588	91.301	188.581	1.00	51.86
	4924	CB	HIS	D	528	67.337	91.112	187.275	1.00	37.99
	4925	CG	HIS	D	528	66.459	90.762	186.118	1.00	60.26
	4926	CD2	HIS	D	528	65.631	89.713	185.908	1.00	94.26
	4927	ND1	HIS	D	528	66.402	91.528	184.973	1.00	110.60
	4928	CE1	HIS	D	528	65.580	90.963	184.107	1.00	110.22
	4929	NE2	HIS	D	528	65.099	89.860	184.651	1.00	125.81
	4930	C	HIS	D	528	66.106	89.963	189.080	1.00	60.71
	4931	O	HIS	D	528	66.741	89.363	189.953	1.00	64.08
	4932	N	GLU	D	529	64.979	89.512	188.533	1.00	75.37
	4933	CA	GLU	D	529	64.388	88.250	188.933	1.00	104.01
	4934	CB	GLU	D	529	63.007	88.110	188.318	1.00	133.95
	4935	CG	GLU	D	529	62.316	86.852	188.709	1.00	183.70
	4936	CD	GLU	D	529	60.964	86.726	188.018	1.00	202.90
	4937	OE1	GLU	D	529	60.677	87.124	186.972	1.00	204.87
	4938	OE2	GLU	D	529	59.987	86.193	188.379	1.00	194.88
	4939	C	GLU	D	529	65.266	87.069	188.541	1.00	117.67
	4940	O	GLU	D	529	65.146	85.986	189.117	1.00	105.24
	4941	N	ALA	D	530	66.198	87.305	187.616	1.00	104.62
	4942	CA	ALA	D	530	67.094	86.252	187.128	1.00	119.79
	4943	CB	ALA	D	530	67.429	86.491	185.653	1.00	110.35
	4944	C	ALA	D	530	68.381	86.118	187.923	1.00	142.01
	4945	O	ALA	D	530	68.445	85.370	188.898	1.00	165.83
	4946	N	ALA	D	531	69.398	86.844	187.473	1.00	133.84
	4947	CA	ALA	D	531	70.724	86.868	188.083	1.00	167.12

	4948	CB	ALA	D	531	71.135	88.308	188.325	1.00	130.57
	4949	C	ALA	D	531	70.905	86.066	189.370	1.00	184.40
	4950	O	ALA	D	531	70.099	86.152	190.298	1.00	180.48
	4951	N	SER	D	532	71.985	85.294	189.421	1.00	188.26
5	4952	CA	SER	D	532	72.294	84.494	190.596	1.00	165.83
	4953	CB	SER	D	532	72.587	83.041	190.197	1.00	154.95
	4954	OG	SER	D	532	71.402	82.364	189.812	1.00	130.00
	4955	C	SER	D	532	73.494	85.093	191.329	1.00	145.61
	4956	O	SER	D	532	74.236	85.909	190.775	1.00	131.77
10	4957	N	PRO	D	533	73.700	84.687	192.588	1.00	134.93
	4958	CD	PRO	D	533	74.977	84.898	193.295	1.00	147.80
	4959	CA	PRO	D	533	72.863	83.723	193.308	1.00	118.05
	4960	CB	PRO	D	533	73.891	82.890	194.044	1.00	151.25
	4961	CG	PRO	D	533	74.856	83.964	194.501	1.00	159.03
15	4962	C	PRO	D	533	71.913	84.426	194.272	1.00	133.53
	4963	O	PRO	D	533	70.971	83.824	194.796	1.00	89.86
	4964	N	SER	D	534	72.180	85.709	194.496	1.00	145.54
	4965	CA	SER	D	534	71.391	86.530	195.406	1.00	131.75
	4966	CB	SER	D	534	72.330	87.327	196.311	1.00	161.36
20	4967	OG	SER	D	534	73.274	88.055	195.538	1.00	169.84
	4968	C	SER	D	534	70.454	87.488	194.679	1.00	120.79
	4969	O	SER	D	534	70.006	88.477	195.250	1.00	109.78
	4970	N	GLN	D	535	70.162	87.192	193.419	1.00	127.46
	4971	CA	GLN	D	535	69.280	88.032	192.618	1.00	106.83
25	4972	CB	GLN	D	535	67.887	88.057	193.244	1.00	30.80
	4973	CG	GLN	D	535	67.263	86.683	193.338	1.00	63.61
	4974	CD	GLN	D	535	66.841	86.320	194.746	1.00	103.06
	4975	OE1	GLN	D	535	67.579	86.550	195.703	1.00	120.06
	4976	NE2	GLN	D	535	65.654	85.735	194.881	1.00	119.16
30	4977	C	GLN	D	535	69.834	89.450	192.454	1.00	81.50
	4978	O	GLN	D	535	69.127	90.369	192.039	1.00	62.58
	4979	N	THR	D	536	71.117	89.603	192.769	1.00	77.55
	4980	CA	THR	D	536	71.818	90.876	192.651	1.00	78.91
	4981	CB	THR	D	536	72.502	91.241	193.964	1.00	101.54
35	4982	OG1	THR	D	536	71.513	91.416	194.980	1.00	139.48
	4983	CG2	THR	D	536	73.313	92.511	193.812	1.00	91.85
	4984	C	THR	D	536	72.908	90.769	191.583	1.00	88.04
	4985	O	THR	D	536	73.332	89.672	191.225	1.00	115.17
	4986	N	VAL	D	537	73.368	91.914	191.092	1.00	73.07
40	4987	CA	VAL	D	537	74.415	91.965	190.078	1.00	83.98
	4988	CB	VAL	D	537	73.851	91.681	188.687	1.00	56.48
	4989	CG1	VAL	D	537	74.764	92.252	187.629	1.00	76.12
	4990	CG2	VAL	D	537	73.701	90.191	188.490	1.00	116.74
	4991	C	VAL	D	537	75.041	93.348	190.075	1.00	97.13
45	4992	O	VAL	D	537	74.349	94.346	189.894	1.00	104.54
	4993	N	GLN	D	538	76.350	93.415	190.263	1.00	95.87
	4994	CA	GLN	D	538	77.004	94.713	190.296	1.00	90.43
	4995	CB	GLN	D	538	77.204	95.139	191.756	1.00	92.33
	4996	CG	GLN	D	538	77.904	94.094	192.622	1.00	78.35
50	4997	CD	GLN	D	538	77.775	94.382	194.105	1.00	103.51
	4998	OE1	GLN	D	538	76.736	94.108	194.715	1.00	86.43
	4999	NE2	GLN	D	538	78.829	94.950	194.695	1.00	114.86
	5000	C	GLN	D	538	78.329	94.733	189.554	1.00	78.31
	5001	O	GLN	D	538	78.903	93.684	189.271	1.00	92.93
55	5002	N	ARG	D	539	78.794	95.936	189.229	1.00	52.71

	5003	CA	ARG	D	539	80.060	96.120	188.539	1.00	93.72
	5004	CB	ARG	D	539	79.846	96.340	187.042	1.00	98.94
	5005	CG	ARG	D	539	81.128	96.234	186.207	1.00	143.16
	5006	CD	ARG	D	539	81.220	94.892	185.479	1.00	155.59
5	5007	NE	ARG	D	539	80.795	93.779	186.324	1.00	160.22
	5008	CZ	ARG	D	539	80.719	92.516	185.921	1.00	144.73
	5009	NH1	ARG	D	539	81.046	92.195	184.678	1.00	164.97
	5010	NH2	ARG	D	539	80.302	91.578	186.760	1.00	105.83
	5011	C	ARG	D	539	80.713	97.352	189.131	1.00	116.29
10	5012	O	ARG	D	539	80.119	98.424	189.130	1.00	77.60
	5013	N	ALA	D	540	81.933	97.195	189.634	1.00	123.66
	5014	CA	ALA	D	540	82.664	98.303	190.232	1.00	90.79
	5015	CB	ALA	D	540	83.843	97.768	191.030	1.00	120.12
	5016	C	ALA	D	540	83.155	99.291	189.179	1.00	83.01
15	5017	O	ALA	D	540	83.133	99.004	187.988	1.00	116.07
	5018	N	VAL	D	541	83.596	100.459	189.629	1.00	73.02
	5019	CA	VAL	D	541	84.107	101.491	188.735	1.00	89.93
	5020	CB	VAL	D	541	82.963	102.295	188.111	1.00	88.65
	5021	CG1	VAL	D	541	82.228	103.037	189.197	1.00	84.77
20	5022	CG2	VAL	D	541	83.498	103.274	187.069	1.00	53.86
	5023	C	VAL	D	541	84.979	102.443	189.547	1.00	102.56
	5024	O	VAL	D	541	85.129	102.267	190.755	1.00	153.42
	5025	N	SER	D	542	85.550	103.446	188.882	1.00	109.91
	5026	CA	SER	D	542	86.397	104.444	189.533	1.00	97.55
25	5027	CB	SER	D	542	87.392	103.773	190.490	1.00	113.18
	5028	OG	SER	D	542	88.174	102.799	189.819	1.00	118.66
	5029	C	SER	D	542	87.169	105.273	188.516	1.00	76.47
	5030	O	SER	D	542	87.411	104.831	187.395	1.00	131.73
	5031	N	VAL	D	543	87.548	106.481	188.909	1.00	61.96
30	5032	CA	VAL	D	543	88.325	107.348	188.034	1.00	111.23
	5033	CB	VAL	D	543	88.073	108.846	188.322	1.00	129.59
	5034	CG1	VAL	D	543	88.348	109.653	187.057	1.00	63.37
	5035	CG2	VAL	D	543	86.642	109.072	188.868	1.00	29.47
	5036	C	VAL	D	543	89.805	107.068	188.309	1.00	152.73
35	5037	O	VAL	D	543	90.167	106.634	189.406	1.00	171.72
	5038	N	ASN	D	544	90.655	107.326	187.320	1.00	149.81
	5039	CA	ASN	D	544	92.091	107.096	187.461	1.00	158.60
	5040	CB	ASN	D	544	92.644	107.880	188.658	1.00	160.72
	5041	CG	ASN	D	544	92.354	109.369	188.568	1.00	151.01
40	5042	OD1	ASN	D	544	92.701	110.027	187.586	1.00	153.71
	5043	ND2	ASN	D	544	91.716	109.907	189.600	1.00	105.81
	5044	C	ASN	D	544	92.415	105.605	187.627	1.00	162.71
	5045	O	ASN	D	544	93.206	105.090	186.810	1.00	168.57
	5046	OXT	ASN	D	544	91.886	104.965	188.563	1.00	91.11
45	5047	C1	NAG	D	694	45.181	116.572	187.768	1.00	63.34
	5048	C2	NAG	D	694	45.182	115.814	186.435	1.00	51.52
	5049	N2	NAG	D	694	43.887	115.931	185.794	1.00	71.95
	5050	C7	NAG	D	694	43.803	116.134	184.485	1.00	76.86
	5051	O7	NAG	D	694	43.995	115.243	183.656	1.00	109.89
50	5052	C8	NAG	D	694	43.455	117.540	184.026	1.00	79.33
	5053	C3	NAG	D	694	45.516	114.334	186.657	1.00	53.42
	5054	O3	NAG	D	694	45.596	113.666	185.403	1.00	84.81
	5055	C4	NAG	D	694	46.845	114.203	187.408	1.00	72.20
	5056	O4	NAG	D	694	47.134	112.810	187.695	1.00	113.39
55	5057	C5	NAG	D	694	46.776	115.015	188.712	1.00	81.05

	5058	O5	NAG	D	694	46.445	116.403	188.432	1.00	76.78
	5059	C6	NAG	D	694	48.102	115.016	189.457	1.00	135.14
	5060	O6	NAG	D	694	49.101	115.734	188.742	1.00	168.86
	5061	C1	NAG	D	695	48.197	112.221	187.004	1.00	162.56
5	5062	C2	NAG	D	695	49.047	111.359	187.959	1.00	161.99
	5063	N2	NAG	D	695	49.643	112.180	188.999	1.00	176.87
	5064	C7	NAG	D	695	49.835	111.675	190.216	1.00	158.22
	5065	O7	NAG	D	695	50.822	111.000	190.511	1.00	158.06
	5066	C8	NAG	D	695	48.769	111.953	191.265	1.00	108.38
10	5067	C3	NAG	D	695	50.146	110.631	187.168	1.00	149.27
	5068	O3	NAG	D	695	50.894	109.785	188.028	1.00	157.06
	5069	C4	NAG	D	695	49.521	109.804	186.043	1.00	139.32
	5070	O4	NAG	D	695	50.565	109.173	185.262	1.00	134.98
	5071	C5	NAG	D	695	48.678	110.741	185.160	1.00	171.70
15	5072	O5	NAG	D	695	47.654	111.397	185.953	1.00	147.36
	5073	C6	NAG	D	695	47.969	110.032	184.022	1.00	163.04
	5074	O6	NAG	D	695	47.105	110.920	183.327	1.00	154.34
	5075	C1	MAN	D	696	50.684	107.790	185.360	1.00	151.20
	5076	C2	MAN	D	696	51.539	107.258	184.202	1.00	196.02
20	5077	O2	MAN	D	696	52.807	107.901	184.205	1.00	199.76
	5078	C3	MAN	D	696	51.725	105.743	184.350	1.00	186.47
	5079	O3	MAN	D	696	52.588	105.259	183.329	1.00	168.62
	5080	C4	MAN	D	696	52.308	105.414	185.732	1.00	184.79
	5081	O4	MAN	D	696	52.356	104.004	185.908	1.00	169.18
25	5082	C5	MAN	D	696	51.437	106.043	186.831	1.00	155.53
	5083	O5	MAN	D	696	51.309	107.471	186.616	1.00	152.57
	5084	C6	MAN	D	696	51.972	105.838	188.246	1.00	138.84
	5085	O6	MAN	D	696	53.387	105.694	188.271	1.00	130.94
	5086	C1	CPS	E	101	26.312	116.112	182.219	1.00	5.42
30	5087	C2	CPS	E	101	25.430	116.494	183.392	1.00	42.91
	5088	C3	CPS	E	101	25.569	114.197	184.531	1.00	20.32
	5089	C4	CPS	E	101	25.066	112.803	185.246	1.00	43.57
	5090	C5	CPS	E	101	24.092	113.131	186.307	1.00	40.19
	5091	C6	CPS	E	101	23.154	114.241	185.856	1.00	48.37
35	5092	C7	CPS	E	101	22.219	114.521	186.964	1.00	35.77
	5093	C8	CPS	E	101	22.186	113.112	187.776	1.00	46.50
	5094	C9	CPS	E	101	23.212	112.183	186.927	1.00	21.17
	5095	C10	CPS	E	101	25.033	113.895	187.520	1.00	6.18
	5096	C11	CPS	E	101	26.201	117.156	184.612	1.00	11.25
40	5097	C12	CPS	E	101	25.595	115.700	180.948	1.00	105.46
	5098	C13	CPS	E	101	24.630	116.690	180.447	1.00	51.23
	5099	C14	CPS	E	101	23.589	117.028	181.573	1.00	47.83
	5100	C15	CPS	E	101	24.383	117.491	182.865	1.00	15.76
	5101	C16	CPS	E	101	23.421	117.851	183.910	1.00	38.47
45	5102	C17	CPS	E	101	22.681	116.741	184.654	1.00	63.19
	5103	C18	CPS	E	101	23.637	115.556	185.273	1.00	9.51
	5104	C19	CPS	E	101	24.660	115.277	183.985	1.00	10.09
	5105	C20	CPS	E	101	23.634	111.029	187.910	1.00	16.56
	5106	C21	CPS	E	101	24.712	110.080	187.465	1.00	66.60
50	5107	C22	CPS	E	101	22.307	110.241	188.314	1.00	66.32
	5108	C23	CPS	E	101	22.401	109.119	189.237	1.00	40.09
	5109	O2	CPS	E	101	23.891	116.247	179.167	1.00	70.91
	5110	O3	CPS	E	101	21.848	116.073	183.892	1.00	56.49
	5111	O4	CPS	E	101	24.411	112.252	184.392	1.00	89.45
55	5112	C1	CHA	E	102	30.416	120.373	183.529	1.00	52.35

	5113	C2	CHA	E	102	29.113	120.721	182.838	1.00	60.47
	5114	C3	CHA	E	102	29.802	119.956	180.443	1.00	57.28
	5115	C4	CHA	E	102	30.034	120.057	178.819	1.00	61.04
	5116	C5	CHA	E	102	28.820	120.636	178.155	1.00	63.59
5	5117	C6	CHA	E	102	28.187	121.729	178.965	1.00	68.16
	5118	C7	CHA	E	102	26.964	122.165	178.185	1.00	71.21
	5119	C8	CHA	E	102	27.365	121.780	176.626	1.00	72.34
	5120	C9	CHA	E	102	28.850	121.169	176.840	1.00	68.39
	5121	C10	CHA	E	102	27.634	119.363	178.205	1.00	37.85
10	5122	C11	CHA	E	102	28.076	119.543	182.924	1.00	58.04
	5123	C12	CHA	E	102	31.426	121.484	183.528	1.00	61.79
	5124	C13	CHA	E	102	30.933	122.729	184.176	1.00	64.51
	5125	C14	CHA	E	102	29.611	123.203	183.499	1.00	70.75
	5126	C15	CHA	E	102	28.577	121.993	183.504	1.00	67.54
15	5127	C16	CHA	E	102	27.325	122.461	182.894	1.00	75.83
	5128	C17	CHA	E	102	27.241	122.710	181.390	1.00	74.20
	5129	C18	CHA	E	102	27.880	121.531	180.440	1.00	63.18
	5130	C19	CHA	E	102	29.262	121.064	181.304	1.00	59.69
	5131	C20	CHA	E	102	29.225	120.329	175.558	1.00	70.63
20	5132	C21	CHA	E	102	30.563	119.632	175.630	1.00	85.68
	5133	C22	CHA	E	102	29.152	121.269	174.231	1.00	65.66
	5134	C23	CHA	E	102	29.532	120.583	172.993	1.00	60.28
	5135	O2	CHA	E	102	31.918	123.917	184.175	1.00	72.67
	5136	O3	CHA	E	102	27.885	123.807	181.001	1.00	76.62
25	5137	O4	CHA	E	102	30.868	120.933	178.735	1.00	61.67
	5138	C24	CHA	E	102	30.917	120.626	172.750	1.00	70.84
	5139	O5	CHA	E	102	31.747	121.244	173.427	1.00	86.94
	5140	N25	CHA	E	102	31.345	119.924	171.722	1.00	71.63
	5141	C25	CHA	E	102	35.585	118.656	169.928	1.00	97.77
30	5142	C26	CHA	E	102	37.184	119.547	171.582	1.00	101.45
	5143	C27	CHA	E	102	32.967	119.825	171.396	1.00	81.57
	5144	C28	CHA	E	102	33.756	119.017	172.519	1.00	73.52
	5145	C29	CHA	E	102	35.099	118.469	172.437	1.00	83.76
	5146	N1	CHA	E	102	36.183	118.470	171.311	1.00	101.30
35	5147	C30	CHA	E	102	36.851	117.076	171.401	1.00	103.79
	5148	C31	CHA	E	102	37.861	116.562	172.339	1.00	103.99
	5149	C32	CHA	E	102	38.216	115.072	172.105	1.00	101.66
	5150	S1	CHA	E	102	37.044	114.052	172.308	1.00	98.10
	5151	O6	CHA	E	102	37.726	112.791	172.029	1.00	94.90
40	5152	O7	CHA	E	102	36.530	114.113	173.536	1.00	94.04
	5153	O8	CHA	E	102	36.102	114.281	171.234	1.00	98.37
	5154	C1	CPS	E	103	32.216	113.269	184.109	1.00	78.09
	5155	C2	CPS	E	103	30.907	113.504	184.849	1.00	57.43
	5156	C3	CPS	E	103	31.645	115.680	185.963	1.00	11.62
45	5157	C4	CPS	E	103	31.940	116.766	187.130	1.00	85.58
	5158	C5	CPS	E	103	30.773	116.851	188.064	1.00	75.94
	5159	C6	CPS	E	103	30.148	115.491	188.287	1.00	54.40
	5160	C7	CPS	E	103	29.007	115.648	189.227	1.00	38.04
	5161	C8	CPS	E	103	29.435	116.990	190.053	1.00	99.76
50	5162	C9	CPS	E	103	30.861	117.406	189.365	1.00	99.01
	5163	C10	CPS	E	103	29.523	117.654	187.165	1.00	26.64
	5164	C11	CPS	E	103	29.830	114.271	183.974	1.00	86.48
	5165	C12	CPS	E	103	33.215	112.383	184.837	1.00	41.22
	5166	C13	CPS	E	103	32.685	111.063	185.227	1.00	35.35
55	5167	C14	CPS	E	103	31.396	111.225	186.094	1.00	60.04

	5168	C15	CPS	E	103	30.372	112.125	185.283	1.00	60.63
	5169	C16	CPS	E	103	29.149	112.239	186.070	1.00	26.81
	5170	C17	CPS	E	103	29.099	113.110	187.300	1.00	68.24
	5171	C18	CPS	E	103	29.746	114.600	187.134	1.00	25.03
5	5172	C19	CPS	E	103	31.088	114.294	186.172	1.00	47.93
	5173	C20	CPS	E	103	31.120	118.945	189.692	1.00	143.80
	5174	C21	CPS	E	103	32.295	119.650	189.055	1.00	182.24
	5175	C22	CPS	E	103	31.182	119.088	191.263	1.00	162.60
	5176	C23	CPS	E	103	31.415	120.407	191.794	1.00	169.03
10	5177	O2	CPS	E	103	33.678	110.186	185.988	1.00	96.90
	5178	O3	CPS	E	103	29.754	112.603	188.293	1.00	39.74
	5179	O4	CPS	E	103	32.821	116.237	187.761	1.00	105.48
	5180	C1	CPS	E	104	20.969	119.198	190.086	1.00	129.45
	5181	C2	CPS	E	104	21.575	119.457	188.703	1.00	48.78
15	5182	C3	CPS	E	104	23.879	120.110	189.583	1.00	31.80
	5183	C4	CPS	E	104	25.238	120.987	189.816	1.00	107.94
	5184	C5	CPS	E	104	25.780	121.443	188.506	1.00	77.04
	5185	C6	CPS	E	104	24.660	121.867	187.572	1.00	43.50
	5186	C7	CPS	E	104	25.269	122.326	186.286	1.00	45.84
20	5187	C8	CPS	E	104	26.760	122.793	186.764	1.00	97.93
	5188	C9	CPS	E	104	26.767	122.465	188.375	1.00	99.02
	5189	C10	CPS	E	104	26.370	119.995	187.748	1.00	36.89
	5190	C11	CPS	E	104	22.163	118.151	188.039	1.00	55.12
	5191	C12	CPS	E	104	20.228	120.384	190.698	1.00	194.25
25	5192	C13	CPS	E	104	19.160	120.964	189.834	1.00	176.18
	5193	C14	CPS	E	104	19.732	121.345	188.421	1.00	77.57
	5194	C15	CPS	E	104	20.460	120.068	187.809	1.00	66.30
	5195	C16	CPS	E	104	20.958	120.428	186.479	1.00	100.76
	5196	C17	CPS	E	104	22.157	121.368	186.362	1.00	79.09
30	5197	C18	CPS	E	104	23.461	120.969	187.291	1.00	12.31
	5198	C19	CPS	E	104	22.712	120.523	188.734	1.00	52.66
	5199	C20	CPS	E	104	28.295	122.305	188.812	1.00	102.44
	5200	C21	CPS	E	104	28.602	121.819	190.202	1.00	40.31
	5201	C22	CPS	E	104	29.033	123.678	188.532	1.00	97.92
35	5202	C23	CPS	E	104	30.441	123.753	188.854	1.00	59.31
	5203	O2	CPS	E	104	18.441	122.194	190.434	1.00	131.97
	5204	O3	CPS	E	104	21.885	122.594	186.735	1.00	102.52
	5205	O4	CPS	E	104	24.841	121.994	190.360	1.00	113.49
	5206	C1	CPS	E	105	23.987	110.282	194.190	1.00	124.07
40	5207	C2	CPS	E	105	23.504	111.201	193.051	1.00	179.02
	5208	C3	CPS	E	105	25.048	113.150	193.677	1.00	146.55
	5209	C4	CPS	E	105	25.528	114.656	194.049	1.00	150.36
	5210	C5	CPS	E	105	24.986	115.634	193.073	1.00	150.31
	5211	C6	CPS	E	105	23.542	115.307	192.719	1.00	151.98
45	5212	C7	CPS	E	105	23.086	116.345	191.744	1.00	129.40
	5213	C8	CPS	E	105	24.069	117.613	192.103	1.00	138.46
	5214	C9	CPS	E	105	25.016	117.025	193.307	1.00	158.19
	5215	C10	CPS	E	105	25.809	115.351	191.555	1.00	57.99
	5216	C11	CPS	E	105	24.253	110.935	191.681	1.00	168.46
50	5217	C12	CPS	E	105	23.199	110.388	195.482	1.00	171.52
	5218	C13	CPS	E	105	21.738	110.182	195.325	1.00	189.12
	5219	C14	CPS	E	105	21.142	111.149	194.226	1.00	180.63
	5220	C15	CPS	E	105	21.981	110.976	192.870	1.00	180.59
	5221	C16	CPS	E	105	21.395	111.864	191.831	1.00	152.08
55	5222	C17	CPS	E	105	21.590	113.385	191.907	1.00	149.04

	5223	C18	CPS	E	105	23.124	113.895	192.254	1.00	131.84
	5224	C19	CPS	E	105	23.632	112.728	193.398	1.00	173.79
	5225	C20	CPS	E	105	26.373	117.881	193.364	1.00	141.17
	5226	C21	CPS	E	105	27.491	117.441	194.289	1.00	61.94
5	5227	C22	CPS	E	105	26.007	119.377	193.665	1.00	163.34
	5228	C23	CPS	E	105	27.114	120.298	193.745	1.00	162.44
	5229	O2	CPS	E	105	20.934	110.337	196.634	1.00	146.47
	5230	O3	CPS	E	105	20.861	113.951	192.840	1.00	182.07
	5231	O4	CPS	E	105	24.940	114.899	195.082	1.00	183.30
10	5232	S	SO4	F	101	26.461	117.594	160.481	1.00	117.04
	5233	O1	SO4	F	101	26.028	117.364	161.888	1.00	114.89
	5234	O2	SO4	F	101	25.645	118.674	159.871	1.00	116.85
	5235	O3	SO4	F	101	27.889	117.990	160.442	1.00	104.02
	5236	O4	SO4	F	101	26.264	116.346	159.701	1.00	116.98
15	5237	S	SO4	F	102	30.691	115.815	152.464	1.00	84.09
	5238	O1	SO4	F	102	31.425	115.760	153.735	1.00	75.95
	5239	O2	SO4	F	102	30.165	117.185	152.282	1.00	88.58
	5240	O3	SO4	F	102	31.591	115.536	151.339	1.00	88.44
	5241	O4	SO4	F	102	29.608	114.799	152.483	1.00	82.42
20	5242	S	SO4	F	103	21.641	101.569	151.307	1.00	92.25
	5243	O1	SO4	F	103	22.530	100.415	151.659	1.00	115.82
	5244	O2	SO4	F	103	21.490	102.482	152.472	1.00	115.45
	5245	O3	SO4	F	103	22.255	102.282	150.149	1.00	112.57
	5246	O4	SO4	F	103	20.304	101.049	150.949	1.00	111.09
25	5247	S	SO4	F	104	63.588	107.320	177.755	1.00	90.55
	5248	O1	SO4	F	104	64.167	105.957	177.946	1.00	104.42
	5249	O2	SO4	F	104	63.018	107.748	179.075	1.00	101.96
	5250	O3	SO4	F	104	64.623	108.285	177.316	1.00	107.44
	5251	O4	SO4	F	104	62.568	107.276	176.668	1.00	101.74
30	5252	S	SO4	F	105	38.290	100.112	181.573	1.00	94.13
	5253	O1	SO4	F	105	39.110	99.271	182.495	1.00	100.20
	5254	O2	SO4	F	105	36.859	99.943	181.952	1.00	108.28
	5255	O3	SO4	F	105	38.642	101.562	181.681	1.00	98.51
	5256	O4	SO4	F	105	38.529	99.646	180.172	1.00	109.17

As used herein, an atomic coordinate, also referred to herein as a structure coordinate or coordinate, is a mathematical coordinate derived from mathematical equations related to the patterns obtained on diffraction of X-rays by the atoms of a protein or complex crystal. The diffraction data are typically used to calculate an electron density map, such as that shown in Fig. 1, which is used to establish the positions of the individual atoms within the unit cell of the crystal. A model that substantially represents the atomic coordinates specified in Table 1 includes not only models that literally represent the coordinates but also models representing a coordinate transformation of such atomic coordinates, for example, by changing the spatial orientation of the coordinates.

The present invention also includes a 3-D model that is a modification of a 3-D model that substantially represents the atomic coordinates specified in Table 1. As used herein, a modification, also referred to herein as a model modification, is a model that represents a complex between a protein that binds to a Fc domain of an antibody and an antibody Fc regon that binds to a Fc receptor protein. A model modification includes, but is not limited to: a refinement of the model that substantially represents the atomic coordinates specified in Table 1; a model representing a complex between any Fc-binding fragment of a Fc receptor protein and any FcR-binding fragment of an antibody having the atomic coordinates specified in Table 1; a model based on other FcεRIα:Fc-Cε3/Cε4 crystals, such as a model based on one or more of the crystals disclosed in the Examples; a model produced using homology modeling techniques to, for example, incorporate all or any part of the amino acid sequence of another FcR or antibody into a 3-D model substantially representing the atomic coordinates specified in Table 1 or incorporate all or

any part of the amino acid sequence of a FcεRIα protein or Fc-Cε3/Cε4 into a 3-D model of a complex between another FcR and antibody; and a modification representing a complex between an FcR and antibody, at least one of which has an altered function, which preferably can be used to design a mutein with an improved function compared to an unmodified protein. As used herein, the term unmodified protein refers to a protein that has not been intentionally subjected to either random or site-directed (i.e., targeted) mutagenesis.

A model of the present invention can be represented in a variety of forms including, but not limited to, listing the coordinates of all atoms comprising the model, providing a physical 3-D model, imaging the model on a computer screen, providing a picture of said model, and deriving a set of coordinates based of a picture of the model, for example by extracting coordinates from a picture or placing a similar immunoglobulin domain into the 3-D model of a human FcεRI$\alpha_{1\text{-}176}$ protein having SEQ ID NO:2 and deriving a model of the similar domain. Physical 3-D models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, Biosym Technologies, San Diego, CA, Tripos, Inc., and Molecular Simulations Inc. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Hard copies include both motion and still pictures. Computer screen images and

pictures of the model can be visualized in a number of formats including, but not limited to, electron density maps, ribbon diagrams, space-filling representations, α carbon traces, topology diagrams, lists of interatomic vectors, phi/psi/chi angle representations of the coordinates, and contact maps, examples of some of which are in the Figs. Representations of the model can include the entire model or portions thereof. A model can also be represented in a database.

A model of the present invention also defines the space surrounding that model. Such a space can be represented as a mold, or alpha-space, that can be used to predict the shape of a compound that inhibits the binding of a FcR and antibody.

In one embodiment, a model of the present invention identifies the solvent accessibility of amino acid residues of the corresponding proteins in the complex. The solvent accessibilities of the amino acids in the complex between PhFcεRIα$_{1\text{-}176mut}$ and PhFc-Cε3/Cε4$_{1\text{-}222}$ are indicated in Table 2.

Table 2. com14i_deposit.pdb Residue Exposure

Surface plot for:
structure file= com14h_gen.mtf
coordinate set= com14i.pdb

				TOTAL ACCESSIBLE AREA		
	segid	resid	resname	residue	mainchain	sidechain
	A	1	VAL	187.3253	57.6982	129.6271
	A	2	PRO	92.7850	27.8208	64.9642
	A	3	GLN	136.0547	22.4120	113.6427
	A	4	LYS	115.4501	16.7110	98.7391
	A	5	PRO	15.6134	5.2823	10.3310
	A	6	LYS	129.5753	2.2724	127.3029
	A	7	VAL	13.2508	10.5326	2.7182
	A	8	SER	61.2891	6.5958	54.6932
	A	9	LEU	29.3720	15.0058	14.3663
	A	10	ASN	96.3611	5.4707	90.8904
	A	11	PRO	61.5816	1.0093	60.5723
	A	12	PRO	44.6585	3.6780	40.9805
	A	13	TRP	32.1306	0.0000	32.1306
	A	14	ASN	13.9201	0.0000	13.9201
	A	15	ARG	18.9379	0.0000	18.9379
	A	16	ILE	4.0671	0.0000	4.0671
	A	17	PHE	2.5761	0.0015	2.5746
	A	18	LYS	75.4097	9.6110	65.7987
	A	19	GLY	30.4736	30.4736	0.0000
	A	20	GLU	38.0623	1.4738	36.5885
	A	21	ASN	44.5154	12.5957	31.9196
	A	22	VAL	6.0341	5.5689	0.4652
	A	23	THR	30.3454	0.0015	30.3439
	A	24	LEU	1.9937	0.0005	1.9933
	A	25	THR	45.1783	0.8036	44.3747
	A	26	CYS	1.8288	1.8288	0.0000
	A	27	ASN	45.5609	16.4355	29.1253
	A	28	GLY	57.0567	57.0567	0.0000
	A	29	ASN	92.9262	33.7771	59.1490
	A	30	ASN	13.5663	9.6698	3.8965
	A	31	PHE	164.0905	20.6501	143.4404
	A	32	PHE	182.6224	29.9619	152.6604
	A	33	GLU	98.9835	23.5598	75.4237
	A	34	VAL	112.1392	35.9284	76.2108
	A	35	SER	13.8929	11.8212	2.0717
	A	36	SER	61.4988	16.1241	45.3747
	A	37	THR	3.8229	1.4419	2.3810
	A	38	LYS	54.6368	1.5373	53.0995
	A	39	TRP	0.7682	0.0026	0.7656
	A	40	PHE	35.2234	0.8384	34.3850
	A	41	HIS	42.4410	4.2641	38.1769
	A	42	ASN	55.8729	34.7289	21.1439
	A	43	GLY	50.2523	50.2523	0.0000
	A	44	SER	90.0908	14.2647	75.8261
	A	45	LEU	112.2293	26.8607	85.3687
	A	46	SER	33.6534	12.6061	21.0473
	A	47	GLU	173.0167	28.6974	144.3194
	A	48	GLU	52.6512	0.9816	51.6696

	A	49	THR	78.9495	4.5450	74.4045
	A	50	ASN	83.8564	1.8107	82.0457
	A	51	SER	20.5641	0.7215	19.8427
	A	52	SER	44.0129	2.6102	41.4027
5	A	53	LEU	23.9390	0.2187	23.7203
	A	54	ASN	93.7074	14.6559	79.0515
	A	55	ILE	14.9901	7.9277	7.0624
	A	56	VAL	77.8026	18.1671	59.6354
	A	57	ASN	72.5436	10.8218	61.7218
10	A	58	ALA	0.1748	0.1748	0.0000
	A	59	LYS	78.3995	0.3905	78.0090
	A	60	PHE	13.8474	0.0000	13.8474
	A	61	GLU	71.1840	0.7867	70.3974
	A	62	ASP	37.6798	0.0000	37.6798
15	A	63	SER	0.7611	0.0000	0.7611
	A	64	GLY	10.5710	10.5710	0.0000
	A	65	GLU	48.7849	0.8856	47.8993
	A	66	TYR	9.3817	0.0000	9.3817
	A	67	LYS	39.4871	0.0208	39.4662
20	A	68	CYS	0.0000	0.0000	0.0000
	A	69	GLN	32.8025	0.0000	32.8025
	A	70	HIS	28.9440	3.7554	25.1886
	A	71	GLN	127.6128	34.5779	93.0349
	A	72	GLN	114.7755	18.7035	96.0721
25	A	73	VAL	129.4891	13.4243	116.0648
	A	74	ALA	32.5769	10.0706	22.5064
	A	75	GLU	64.6775	8.8568	55.8208
	A	76	SER	1.9255	1.8897	0.0358
	A	77	GLU	112.0982	4.5586	107.5397
30	A	78	PRO	50.1437	14.6260	35.5177
	A	79	VAL	26.4528	3.6105	22.8422
	A	80	TYR	121.0925	5.3004	115.7921
	A	81	LEU	1.8512	0.7930	1.0581
	A	82	GLU	59.7116	0.0003	59.7113
35	A	83	VAL	9.5413	9.5413	0.0000
	A	84	PHE	35.6448	3.2623	32.3825
	A	85	SER	24.8318	9.3417	15.4901
	A	86	ASP	22.6050	0.0005	22.6045
	A	87	TRP	25.2208	0.6392	24.5816
40	A	88	LEU	3.0061	3.0061	0.0000
	A	89	LEU	4.7629	1.9707	2.7922
	A	90	LEU	0.6339	0.6339	0.0000
	A	91	GLN	0.7211	0.0000	0.7211
	A	92	ALA	1.9224	0.9484	0.9739
45	A	93	SER	28.3506	16.9666	11.3840
	A	94	ALA	31.9213	3.2557	28.6657
	A	95	GLU	59.5399	4.5153	55.0246
	A	96	VAL	90.3253	19.0678	71.2575
	A	97	VAL	6.3340	1.9033	4.4307
50	A	98	MET	117.6508	1.1378	116.5130
	A	99	GLU	87.6346	20.1858	67.4487
	A	100	GLY	37.5111	37.5111	0.0000
	A	101	GLN	86.3207	1.7512	84.5695
	A	102	PRO	60.8738	6.3890	54.4848
55	A	103	LEU	0.4221	0.0000	0.4221

	A	104	PHE	80.0346	0.0026	80.0320
	A	105	LEU	0.1253	0.1242	0.0011
	A	106	ARG	68.1925	0.0000	68.1925
	A	107	CYS	3.4779	3.4779	0.0000
5	A	108	HIS	11.8995	0.9286	10.9708
	A	109	GLY	3.1287	3.1287	0.0000
	A	110	TRP	32.3303	0.5358	31.7945
	A	111	ARG	102.0115	29.5393	72.4722
	A	112	ASN	103.7825	16.7021	87.0804
10	A	113	TRP	8.0187	5.9544	2.0643
	A	114	ASP	56.0982	5.8709	50.2273
	A	115	VAL	3.8019	3.8019	0.0000
	A	116	TYR	28.0985	0.0025	28.0959
	A	117	LYS	13.8640	4.0420	9.8220
15	A	118	VAL	0.0000	0.0000	0.0000
	A	119	ILE	2.9639	0.0000	2.9639
	A	120	TYR	0.0664	0.0000	0.0664
	A	121	TYR	33.2837	0.0000	33.2837
	A	122	LYS	25.5895	0.0240	25.5655
20	A	123	ASP	78.1271	25.4180	52.7091
	A	124	GLY	62.3032	62.3032	0.0000
	A	125	GLU	120.1814	5.1946	114.9868
	A	126	ALA	31.3601	27.4382	3.9219
	A	127	LEU	76.9250	25.4102	51.5147
25	A	128	LYS	112.4216	4.4777	107.9440
	A	129	TYR	5.7182	5.6069	0.1112
	A	130	TRP	71.2318	0.0019	71.2299
	A	131	TYR	2.3182	1.8150	0.5032
	A	132	GLU	48.8765	0.0000	48.8765
30	A	133	ASN	56.4646	18.4026	38.0620
	A	134	HIS	34.7605	14.3500	20.4105
	A	135	ALA	61.0033	21.2841	39.7192
	A	136	ILE	12.9140	2.0093	10.9047
	A	137	SER	71.4379	27.1612	44.2767
35	A	138	ILE	24.6119	3.4516	21.1603
	A	139	THR	103.9450	8.8762	95.0688
	A	140	ASN	102.3330	12.7166	89.6164
	A	141	ALA	10.3600	10.0810	0.2790
	A	142	ALA	34.0280	8.3960	25.6320
40	A	143	VAL	104.7568	10.1018	94.6550
	A	144	GLU	126.9246	18.8779	108.0467
	A	145	ASP	16.9194	0.0000	16.9194
	A	146	SER	21.5373	4.0635	17.4739
	A	147	GLY	5.8021	5.8021	0.0000
45	A	148	THR	32.5295	0.0829	32.4466
	A	149	TYR	0.0642	0.0000	0.0642
	A	150	TYR	43.8958	0.0226	43.8733
	A	151	CYS	0.0000	0.0000	0.0000
	A	152	THR	29.2303	0.0000	29.2303
50	A	153	GLY	3.9813	3.9813	0.0000
	A	154	LYS	48.4892	0.3347	48.1546
	A	155	VAL	2.0858	0.5817	1.5040
	A	156	TRP	18.7900	7.0495	11.7404
	A	157	GLN	31.8404	12.3565	19.4840
55	A	158	LEU	36.5178	1.3940	35.1238

	A	159	ASP	102.6316	23.8299	78.8017
	A	160	TYR	48.3992	8.9529	39.4463
	A	161	GLU	105.3209	20.1949	85.1260
	A	162	SER	3.4294	3.2706	0.1588
5	A	163	GLU	82.4632	5.8768	76.5864
	A	164	PRO	93.8712	16.5130	77.3582
	A	165	LEU	14.1332	2.3506	11.7826
	A	166	ASN	40.8356	7.7631	33.0724
	A	167	ILE	1.0917	1.0901	0.0016
10	A	168	THR	60.5937	0.4273	60.1664
	A	169	VAL	30.1152	27.9591	2.1560
	A	170	ILE	90.8904	5.5150	85.3753
	A	171	LYS	136.7114	19.0209	117.6905
	A	172	ALA	86.7389	24.6924	62.0465
15	A	173	PRO	192.4729	58.6006	133.8723
	A	221	NAG	140.3112	0.0000	140.3112
	A	222	NAG	177.5229	0.0000	177.5229
	A	223	MAN	225.6042	0.0000	225.6042
	A	224	FUC	193.3727	0.0000	193.3727
20	A	242	NAG	142.0058	0.0000	142.0058
	A	243	NAG	139.1866	0.0000	139.1866
	A	244	MAN	61.6458	0.0000	61.6458
	A	245	MAN	221.3300	0.0000	221.3300
	A	246	MAN	162.9047	0.0000	162.9047
25	A	366	NAG	163.0167	0.0000	163.0167
	A	367	NAG	271.0832	0.0000	271.0832
	A	369	FUC	170.1425	0.0000	170.1425
	B	328	PRO	172.3911	55.4048	116.9864
	B	329	CYS	28.4788	7.8618	20.6170
30	B	330	ASP	92.8612	15.7041	77.1570
	B	331	SER	27.0273	1.1252	25.9021
	B	332	ASN	34.9448	0.0015	34.9432
	B	333	PRO	0.0000	0.0000	0.0000
	B	334	ARG	56.1569	7.6844	48.4725
35	B	335	GLY	1.1847	1.1847	0.0000
	B	336	VAL	0.0012	0.0012	0.0000
	B	337	SER	15.0140	0.0510	14.9630
	B	338	ALA	5.2899	4.7848	0.5050
	B	339	TYR	51.0452	3.6676	47.3776
40	B	340	LEU	29.3001	25.9417	3.3584
	B	341	SER	45.2273	8.8444	36.3829
	B	342	ARG	88.6974	12.2167	76.4807
	B	343	PRO	8.9769	8.9769	0.0000
	B	344	SER	38.4813	6.2806	32.2008
45	B	345	PRO	14.1279	3.1946	10.9334
	B	346	PHE	47.7276	0.0000	47.7276
	B	347	ASP	47.1591	0.0000	47.1591
	B	348	LEU	7.6413	0.3974	7.2439
	B	349	PHE	17.8265	8.5197	9.3068
50	B	350	ILE	46.3116	12.5396	33.7719
	B	351	ARG	138.4411	22.8644	115.5766
	B	352	LYS	138.7623	15.9014	122.8608
	B	353	SER	48.1246	7.3438	40.7808
	B	354	PRO	3.8128	1.3726	2.4402
55	B	355	THR	55.0488	11.3329	43.7158

	B	356	ILE	0.4059	0.4059	0.0000
	B	357	THR	39.8398	1.4897	38.3501
	B	358	CYS	0.3982	0.0000	0.3982
	B	359	LEU	21.2325	0.0000	21.2325
5	B	360	VAL	0.6920	0.0000	0.6920
	B	361	VAL	0.7258	0.0000	0.7258
	B	362	ASP	6.8200	0.2493	6.5707
	B	363	LEU	4.2335	0.0000	4.2335
	B	364	ALA	3.3493	2.6950	0.6543
10	B	365	PRO	82.6759	12.6105	70.0654
	B	366	SER	50.6093	40.2181	10.3912
	B	367	LYS	213.9320	43.2881	170.6439
	B	368	GLY	40.8947	40.8947	0.0000
	B	369	THR	86.8598	19.7007	67.1591
15	B	370	VAL	15.5137	7.3337	8.1800
	B	371	ASN	81.8915	3.4400	78.4515
	B	372	LEU	22.8095	18.5551	4.2544
	B	373	THR	63.4928	3.2688	60.2240
	B	374	TRP	23.4425	13.9341	9.5085
20	B	375	SER	45.2542	3.8130	41.4412
	B	376	ARG	46.0272	18.4454	27.5818
	B	377	ALA	72.9508	41.9432	31.0077
	B	378	SER	61.4249	42.7807	18.6442
	B	379	GLY	62.6791	62.6791	0.0000
25	B	380	LYS	117.6325	4.9136	112.7189
	B	381	PRO	121.4544	18.6968	102.7576
	B	382	VAL	56.2720	27.9106	28.3614
	B	383	ASN	91.2257	9.8352	81.3905
	B	384	HIS	171.4010	14.9519	156.4491
30	B	385	SER	60.0998	34.1545	25.9453
	B	386	THR	61.8510	7.3810	54.4700
	B	387	ARG	90.5383	34.3831	56.1553
	B	388	LYS	116.7691	6.8649	109.9042
	B	389	GLU	68.1229	29.0561	39.0668
35	B	390	GLU	95.8196	5.5952	90.2244
	B	391	LYS	165.8039	23.0467	142.7572
	B	392	GLN	28.9793	6.2030	22.7763
	B	393	ARG	216.3236	21.7321	194.5916
	B	394	ASN	21.4124	2.2263	19.1861
40	B	395	GLY	18.5421	18.5421	0.0000
	B	396	THR	1.4681	0.8446	0.6234
	B	397	LEU	27.8812	0.0001	27.8811
	B	398	THR	2.5805	0.0070	2.5735
	B	399	VAL	0.2989	0.0000	0.2989
45	B	400	THR	28.7559	0.0010	28.7549
	B	401	SER	1.6019	0.0320	1.5699
	B	402	THR	38.8714	1.4031	37.4684
	B	403	LEU	1.4485	0.0026	1.4459
	B	404	PRO	54.7046	5.1244	49.5802
50	B	405	VAL	9.9534	9.2686	0.6848
	B	406	GLY	19.5973	19.5973	0.0000
	B	407	THR	17.5422	0.0269	17.5153
	B	408	ARG	149.2990	4.0416	145.2574
	B	409	ASP	50.9581	6.4926	44.4655
55	B	410	TRP	13.6629	0.0000	13.6629

	B	411	ILE	58.9623	7.5292	51.4331
	B	412	GLU	150.4506	36.6377	113.8129
	B	413	GLY	37.5912	37.5912	0.0000
	B	414	GLU	20.7783	6.9542	13.8241
5	B	415	THR	41.3262	0.7425	40.5837
	B	416	TYR	9.7756	0.0127	9.7629
	B	417	GLN	62.7741	0.0234	62.7507
	B	418	CYS	0.5661	0.4620	0.1041
	B	419	ARG	116.8504	0.4330	116.4174
10	B	420	VAL	3.0810	0.0024	3.0786
	B	421	THR	53.9214	2.2639	51.6575
	B	422	HIS	11.9613	3.7559	8.2055
	B	423	PRO	118.2970	36.7814	81.5157
	B	424	HIS	41.1729	9.3203	31.8526
15	B	425	LEU	20.1433	18.3272	1.8162
	B	426	PRO	95.2197	47.9729	47.2468
	B	427	ARG	75.8053	12.6035	63.2017
	B	428	ALA	29.9192	13.4376	16.4816
	B	429	LEU	0.6655	0.2491	0.4164
20	B	430	MET	94.7862	13.9214	80.8648
	B	431	ARG	61.2436	10.0257	51.2179
	B	432	SER	65.6617	25.5585	40.1032
	B	433	THR	13.0233	5.6973	7.3260
	B	434	THR	46.6839	7.5817	39.1022
25	B	435	LYS	48.5670	13.2907	35.2763
	B	436	THR	47.1262	7.7492	39.3770
	B	437	SER	93.7617	15.6507	78.1110
	B	438	GLY	47.1648	47.1648	0.0000
	B	439	PRO	92.2539	11.4315	80.8224
30	B	440	ARG	86.4119	32.6025	53.8094
	B	441	ALA	41.0049	5.6703	35.3346
	B	442	ALA	46.7251	10.6945	36.0306
	B	443	PRO	4.7646	4.7646	0.0000
	B	444	GLU	32.6629	0.1921	32.4708
35	B	445	VAL	1.9628	0.1088	1.8541
	B	446	TYR	12.1809	1.1154	11.0655
	B	447	ALA	19.0771	18.8089	0.2682
	B	448	PHE	32.2261	5.3355	26.8906
	B	449	ALA	26.3527	17.5706	8.7821
40	B	450	THR	8.1738	2.2896	5.8842
	B	451	PRO	76.5842	4.9904	71.5938
	B	452	GLU	93.8169	13.0331	80.7838
	B	453	TRP	95.9141	1.6990	94.2151
	B	454	PRO	125.8288	36.9609	88.8679
45	B	455	GLY	65.7610	65.7610	0.0000
	B	456	SER	42.7528	8.4299	34.3229
	B	457	ARG	182.0093	19.8205	162.1888
	B	458	ASP	66.4899	1.5486	64.9413
	B	459	LYS	148.5472	12.9959	135.5513
50	B	460	ARG	41.5604	3.1133	38.4471
	B	461	THR	13.2538	1.6604	11.5934
	B	462	LEU	6.3258	0.0649	6.2610
	B	463	ALA	11.5779	0.4739	11.1040
	B	464	CYS	1.0391	1.0391	0.0000
55	B	465	LEU	2.3588	0.0000	2.3588

	B	466	ILE	0.3683	0.0000	0.3683
	B	467	GLN	4.2086	0.0000	4.2086
	B	468	ASN	35.9496	5.2065	30.7431
	B	469	PHE	0.0000	0.0000	0.0000
5	B	470	MET	32.7360	0.0000	32.7360
	B	471	PRO	9.7948	6.3053	3.4896
	B	472	GLU	88.4549	3.7638	84.6910
	B	473	ASP	47.2351	6.8458	40.3893
	B	474	ILE	29.1817	24.1296	5.0520
10	B	475	SER	14.3571	4.1523	10.2049
	B	476	VAL	20.6222	18.5324	2.0898
	B	477	GLN	10.6533	0.0000	10.6533
	B	478	TRP	1.8912	1.0361	0.8551
	B	479	LEU	28.2585	0.9455	27.3131
15	B	480	HIS	9.7124	1.2163	8.4961
	B	481	ASN	54.6134	14.8060	39.8074
	B	482	GLU	172.9182	41.2890	131.6292
	B	483	VAL	80.4369	2.9369	77.5000
	B	484	GLN	86.7995	23.2392	63.5604
20	B	485	LEU	20.1440	8.7226	11.4214
	B	486	PRO	79.3531	10.9230	68.4300
	B	487	ASP	113.7037	8.5271	105.1766
	B	488	ALA	105.1557	42.1652	62.9905
	B	489	ARG	78.5174	20.7364	57.7810
25	B	490	HIS	27.7987	16.2252	11.5735
	B	491	SER	30.5621	5.9459	24.6161
	B	492	THR	40.2793	15.9582	24.3211
	B	493	THR	12.2109	4.6417	7.5692
	B	494	GLN	99.8352	2.7394	97.0958
30	B	495	PRO	38.5051	18.8569	19.6482
	B	496	ARG	86.5718	5.6625	80.9093
	B	497	LYS	159.5251	21.1005	138.4247
	B	498	THR	19.4014	18.8518	0.5496
	B	499	LYS	201.9754	42.6147	159.3607
35	B	500	GLY	44.4883	44.4883	0.0000
	B	501	SER	85.5433	25.6861	59.8572
	B	502	GLY	1.9867	1.9867	0.0000
	B	503	PHE	31.1871	0.0000	31.1871
	B	504	PHE	1.5596	0.0598	1.4998
40	B	505	VAL	0.9708	0.0000	0.9708
	B	506	PHE	3.7613	0.1850	3.5763
	B	507	SER	0.6262	0.0195	0.6068
	B	508	ARG	9.5731	1.8218	7.7513
	B	509	LEU	0.7046	0.0000	0.7046
45	B	510	GLU	62.9883	2.0494	60.9388
	B	511	VAL	10.8762	6.5365	4.3397
	B	512	THR	71.0071	0.0263	70.9809
	B	513	ARG	104.2393	0.0000	104.2393
	B	514	ALA	65.4206	13.1707	52.2499
50	B	515	GLU	35.3933	0.3618	35.0315
	B	516	TRP	39.6550	3.3357	36.3193
	B	517	GLU	115.3847	37.2436	78.1411
	B	518	GLN	113.6505	33.6727	79.9778
	B	519	LYS	84.0921	8.7130	75.3791
55	B	520	ASP	64.5129	2.3376	62.1754

	B	521	GLU	87.5584	2.3918	85.1666
	B	522	PHE	9.6600	0.0000	9.6600
	B	523	ILE	30.2820	0.0000	30.2820
	B	524	CYS	0.0000	0.0000	0.0000
5	B	525	ARG	37.1783	0.0000	37.1783
	B	526	ALA	0.3818	0.3818	0.0000
	B	527	VAL	0.0418	0.0000	0.0418
	B	528	HIS	0.6191	0.1432	0.4759
	B	529	GLU	49.1816	17.5861	31.5955
10	B	530	ALA	25.6926	20.8074	4.8853
	B	531	ALA	7.1284	6.1152	1.0132
	B	532	SER	92.9571	24.3505	68.6065
	B	533	PRO	129.7170	30.9019	98.8150
	B	534	SER	65.6135	12.1706	53.4428
15	B	535	GLN	60.5061	0.0227	60.4835
	B	536	THR	22.1684	5.5560	16.6125
	B	537	VAL	29.6659	6.3253	23.3407
	B	538	GLN	69.4992	13.4096	56.0896
	B	539	ARG	92.2922	3.4257	88.8665
20	B	540	ALA	62.4168	19.4066	43.0101
	B	541	VAL	19.1443	12.3199	6.8244
	B	542	SER	49.6556	19.3884	30.2672
	B	543	VAL	20.6069	2.0847	18.5222
	B	544	ASN	178.7782	70.1438	108.6343
25	B	694	NAG	107.4774	0.0000	107.4774
	B	695	NAG	119.4719	0.0000	119.4719
	B	696	MAN	45.7067	0.0000	45.7067
	B	697	MAN	152.8463	0.0000	152.8463
	B	698	MAN	222.3243	0.0000	222.3243
30	B	699	MAN	217.3122	0.0000	217.3122
	D	329	CYS	102.3809	67.5332	34.8476
	D	330	ASP	111.3542	32.4992	78.8550
	D	331	SER	49.5069	8.1508	41.3561
	D	332	ASN	19.9483	7.1538	12.7945
35	D	333	PRO	20.7718	9.3148	11.4570
	D	334	ARG	103.0460	10.1992	92.8468
	D	335	GLY	3.3799	3.3799	0.0000
	D	336	VAL	12.9305	10.8477	2.0827
	D	337	SER	17.9779	5.3981	12.5798
40	D	338	ALA	2.9541	2.7192	0.2349
	D	339	TYR	68.8053	3.1433	65.6620
	D	340	LEU	28.1176	26.0926	2.0250
	D	341	SER	59.6285	9.0359	50.5926
	D	342	ARG	87.3522	11.5821	75.7702
45	D	343	PRO	7.5238	7.5238	0.0000
	D	344	SER	36.9529	6.5208	30.4322
	D	345	PRO	11.5386	3.1229	8.4157
	D	346	PHE	45.5005	0.0000	45.5005
	D	347	ASP	47.0584	0.0024	47.0561
50	D	348	LEU	9.0480	0.3353	8.7126
	D	349	PHE	22.9831	9.2421	13.7410
	D	350	ILE	57.3966	13.5038	43.8927
	D	351	ARG	140.1074	22.9695	117.1379
	D	352	LYS	139.7937	14.7242	125.0695
55	D	353	SER	48.1517	7.3618	40.7899

	D	354	PRO	3.2206	0.8205	2.4000
	D	355	THR	54.2972	11.4293	42.8679
	D	356	ILE	0.4144	0.4144	0.0000
	D	357	THR	39.9578	1.7071	38.2507
5	D	358	CYS	0.3097	0.0000	0.3097
	D	359	LEU	18.5271	0.0018	18.5253
	D	360	VAL	1.3679	0.0000	1.3679
	D	361	VAL	0.3469	0.0000	0.3469
	D	362	ASP	12.4469	6.3831	6.0638
10	D	363	LEU	4.9868	1.6440	3.3428
	D	364	ALA	19.9780	5.4292	14.5488
	D	365	PRO	65.0465	6.1738	58.8727
	D	366	SER	32.8048	26.7953	6.0096
	D	367	LYS	136.0098	36.9049	99.1049
15	D	368	GLY	26.7169	26.7169	0.0000
	D	369	THR	93.8010	14.7194	79.0816
	D	370	VAL	15.1817	1.2150	13.9667
	D	371	ASN	71.4877	1.7213	69.7664
	D	372	LEU	27.5581	21.2832	6.2749
20	D	373	THR	64.9412	3.5271	61.4141
	D	374	TRP	21.6411	12.7579	8.8832
	D	375	SER	45.5983	4.0264	41.5719
	D	376	ARG	46.1407	18.3951	27.7456
	D	377	ALA	73.2052	42.7392	30.4661
25	D	378	SER	60.9391	42.2524	18.6867
	D	379	GLY	62.4810	62.4810	0.0000
	D	380	LYS	114.3210	4.9018	109.4192
	D	381	PRO	118.6128	19.3560	99.2568
	D	382	VAL	56.2105	27.7078	28.5027
30	D	383	ASN	89.7140	9.4333	80.2807
	D	384	HIS	175.3907	15.2111	160.1796
	D	385	SER	60.1172	34.0544	26.0628
	D	386	THR	63.3471	6.6705	56.6765
	D	387	ARG	100.5610	32.1288	68.4323
35	D	388	LYS	117.6302	8.3122	109.3179
	D	389	GLU	93.9137	30.6429	63.2707
	D	390	GLU	96.2332	5.9265	90.3067
	D	391	LYS	170.3439	24.4483	145.8956
	D	392	GLN	31.5360	6.5112	25.0248
40	D	393	ARG	229.7092	34.9960	194.7132
	D	394	ASN	71.2822	36.9290	34.3532
	D	395	GLY	54.2216	54.2216	0.0000
	D	396	THR	14.4859	6.7168	7.7691
	D	397	LEU	31.2188	0.0000	31.2188
45	D	398	THR	0.9937	0.0352	0.9584
	D	399	VAL	1.8265	0.0023	1.8242
	D	400	THR	28.8418	0.0000	28.8418
	D	401	SER	1.8342	0.0000	1.8342
	D	402	THR	38.4300	1.3612	37.0688
50	D	403	LEU	1.3700	0.0000	1.3700
	D	404	PRO	56.4630	5.0109	51.4521
	D	405	VAL	10.3785	9.6144	0.7642
	D	406	GLY	19.9415	19.9415	0.0000
	D	407	THR	17.7730	0.0342	17.7388
55	D	408	ARG	149.6237	4.1119	145.5118

	D	409	ASP	52.0866	6.4418	45.6449
	D	410	TRP	13.1899	0.0000	13.1899
	D	411	ILE	63.5723	7.3792	56.1932
	D	412	GLU	148.7782	36.0783	112.6999
5	D	413	GLY	38.9396	38.9396	0.0000
	D	414	GLU	20.8518	6.7344	14.1173
	D	415	THR	39.3540	0.6913	38.6627
	D	416	TYR	5.8935	0.0014	5.8921
	D	417	GLN	62.2903	0.0009	62.2895
10	D	418	CYS	0.4753	0.3779	0.0974
	D	419	ARG	106.4535	0.4475	106.0060
	D	420	VAL	2.7864	0.0595	2.7269
	D	421	THR	47.3939	3.4111	43.9828
	D	422	HIS	13.1471	8.0455	5.1016
15	D	423	PRO	73.2651	38.6918	34.5733
	D	424	HIS	5.0313	3.9403	1.0910
	D	425	LEU	26.2169	16.8989	9.3180
	D	426	PRO	16.7230	16.7230	0.0000
	D	427	ARG	90.3191	7.4734	82.8457
20	D	428	ALA	36.2453	22.9999	13.2454
	D	429	LEU	33.6211	0.8879	32.7333
	D	430	MET	81.2915	16.0381	65.2534
	D	431	ARG	95.2832	10.2332	85.0500
	D	432	SER	62.4521	22.5286	39.9235
25	D	433	THR	16.4152	7.6464	8.7688
	D	434	THR	43.2290	5.7565	37.4725
	D	435	LYS	48.4737	13.5566	34.9171
	D	436	THR	40.0113	7.5864	32.4249
	D	437	SER	92.1976	14.6061	77.5915
30	D	438	GLY	47.1703	47.1703	0.0000
	D	439	PRO	87.5094	11.3492	76.1603
	D	440	ARG	91.1554	32.4332	58.7222
	D	441	ALA	37.6064	5.6168	31.9896
	D	442	ALA	47.7716	10.8839	36.8877
35	D	443	PRO	4.7444	4.7444	0.0000
	D	444	GLU	31.7469	0.2472	31.4997
	D	445	VAL	2.2316	0.4056	1.8260
	D	446	TYR	13.0081	1.2161	11.7920
	D	447	ALA	19.3686	19.1556	0.2130
40	D	448	PHE	32.4618	5.0174	27.4445
	D	449	ALA	26.4564	17.8510	8.6054
	D	450	THR	6.7460	1.4957	5.2504
	D	451	PRO	78.1205	5.0753	73.0452
	D	452	GLU	98.7545	13.9213	84.8332
45	D	453	TRP	95.8047	1.7250	94.0797
	D	454	PRO	125.4561	37.0254	88.4307
	D	455	GLY	65.7398	65.7398	0.0000
	D	456	SER	42.2645	8.7091	33.5554
	D	457	ARG	185.3827	19.6535	165.7292
50	D	458	ASP	64.7836	1.4527	63.3309
	D	459	LYS	150.1746	13.4092	136.7655
	D	460	ARG	41.0497	3.6090	37.4407
	D	461	THR	12.7243	1.3702	11.3540
	D	462	LEU	5.8977	0.0000	5.8977
55	D	463	ALA	9.3450	0.3148	9.0302

	D	464	CYS	0.6992	0.6992	0.0000
	D	465	LEU	2.3713	0.0565	2.3149
	D	466	ILE	0.3495	0.0005	0.3490
	D	467	GLN	5.5766	0.0000	5.5766
5	D	468	ASN	37.3320	5.0478	32.2843
	D	469	PHE	0.0020	0.0020	0.0000
	D	470	MET	31.1122	0.0000	31.1122
	D	471	PRO	7.4404	4.3666	3.0739
	D	472	GLU	83.9660	3.9591	80.0069
10	D	473	ASP	40.3144	6.4854	33.8290
	D	474	ILE	29.6267	24.7486	4.8781
	D	475	SER	15.2528	4.1160	11.1368
	D	476	VAL	20.2396	18.2215	2.0182
	D	477	GLN	12.4429	0.0027	12.4403
15	D	478	TRP	1.7703	0.9849	0.7854
	D	479	LEU	28.1196	1.0451	27.0745
	D	480	HIS	9.4122	1.1137	8.2985
	D	481	ASN	56.0442	16.0061	40.0381
	D	482	GLU	170.6455	41.2302	129.4154
20	D	483	VAL	80.9853	2.7860	78.1993
	D	484	GLN	88.3797	22.1725	66.2072
	D	485	LEU	20.3000	9.0697	11.2303
	D	486	PRO	79.3386	10.6028	68.7358
	D	487	ASP	114.5014	8.7729	105.7285
25	D	488	ALA	104.3458	41.8161	62.5297
	D	489	ARG	79.9265	20.4064	59.5200
	D	490	HIS	27.6480	16.2092	11.4388
	D	491	SER	29.4802	5.4279	24.0523
	D	492	THR	40.7927	16.2337	24.5591
30	D	493	THR	11.8506	4.3668	7.4838
	D	494	GLN	119.5958	2.8589	116.7369
	D	495	PRO	39.1911	18.6929	20.4981
	D	496	ARG	86.9475	5.7213	81.2261
	D	497	LYS	160.3208	19.6386	140.6822
35	D	498	THR	18.7636	18.4350	0.3286
	D	499	LYS	200.0818	42.2517	157.8301
	D	500	GLY	44.5668	44.5668	0.0000
	D	501	SER	86.6338	25.9131	60.7207
	D	502	GLY	1.8767	1.8767	0.0000
40	D	503	PHE	31.3369	0.0034	31.3334
	D	504	PHE	1.4032	0.0633	1.3399
	D	505	VAL	0.8780	0.0000	0.8780
	D	506	PHE	4.3508	0.1793	4.1714
	D	507	SER	0.5298	0.0000	0.5298
45	D	508	ARG	8.9714	1.8540	7.1174
	D	509	LEU	0.7079	0.0000	0.7079
	D	510	GLU	61.8196	1.9056	59.9140
	D	511	VAL	10.8929	6.6139	4.2790
	D	512	THR	71.8291	0.0838	71.7453
50	D	513	ARG	105.1744	0.0000	105.1744
	D	514	ALA	65.9787	13.5900	52.3887
	D	515	GLU	36.2623	0.0481	36.2142
	D	516	TRP	40.1069	3.3758	36.7311
	D	517	GLU	115.7130	37.9922	77.7208
55	D	518	GLN	110.4985	32.2394	78.2591

	D	519	LYS	84.2805	8.6356	75.6448
	D	520	ASP	65.1989	2.2319	62.9670
	D	521	GLU	87.5054	1.9237	85.5818
	D	522	PHE	9.4572	0.0000	9.4572
5	D	523	ILE	31.1442	0.0000	31.1442
	D	524	CYS	0.0003	0.0003	0.0000
	D	525	ARG	39.5175	0.0000	39.5175
	D	526	ALA	0.4314	0.4314	0.0000
	D	527	VAL	0.1473	0.0000	0.1473
10	D	528	HIS	0.6558	0.1273	0.5285
	D	529	GLU	49.3913	17.1907	32.2006
	D	530	ALA	25.8310	20.8648	4.9662
	D	531	ALA	6.3430	5.3376	1.0054
	D	532	SER	90.9851	24.3589	66.6262
15	D	533	PRO	129.9180	31.2948	98.6232
	D	534	SER	63.8534	10.9652	52.8881
	D	535	GLN	62.1692	0.1376	62.0316
	D	536	THR	20.7628	5.8645	14.8983
	D	537	VAL	29.9134	6.1442	23.7692
20	D	538	GLN	73.2944	13.0975	60.1969
	D	539	ARG	94.0071	3.3512	90.6559
	D	540	ALA	62.7499	19.2166	43.5333
	D	541	VAL	20.0580	13.1091	6.9490
	D	542	SER	52.5909	21.4389	31.1520
25	D	543	VAL	20.1018	2.8350	17.2667
	D	544	ASN	177.6491	71.3693	106.2798
	D	694	NAG	136.0235	0.0000	136.0235
	D	695	NAG	128.7899	0.0000	128.7899
	D	696	MAN	176.7398	0.0000	176.7398
30	E	101	CPS	163.2849	0.0000	163.2849
	E	102	CHA	333.1883	0.0000	333.1883
	E	103	CPS	83.0589	0.0000	83.0589
	E	104	CPS	313.3217	0.0000	313.3217
	E	105	CPS	246.4972	0.0000	246.4972

Residues that are solvent accessible are important as they represent amino acids that are on the external surface of the proteins in the complex and, as such, may be involved in binding of a FcR to an antibody and as such be useful in designing proteins with an enhanced binding activity or in identifying compounds that inhibit such binding. In addition, solvent accessible residues can represent targets for modification to produce a FcR or antibody with improved function. Such analysis also identifies residues in the interior, or core, of the proteins in the complex. Such residues can also be targeted to produce proteins with improved functions, such as enhanced stability.

A model of the present invention also provides additional information that is not available from other sources. For example, a model can identify the crystal contacts between crystals and predict the location of the IgE binding domain, including those amino acids that actually form contacts with a Fc domain of an IgE antibody, such as those in the binding face of the FcεRIα protein. A model can also identify the amino acids in the interface between domain 1 and domain 2 (i.e., the D1D2 interface), as well as those in the cleft formed between the two domains of the FcεRIα protein. Particularly important regions of the complex indicated by the model represented in Table 1 include, but are not limited to, FcεRIα:Fc-Cε3/Cε4 interaction site 1, FcεRIα:Fc-Cε3/Cε4 interaction site 2, the hinge between domain Cε3 and domain Cε4 of the Fc-Cε3/Cε4 region, and a FcεRIα:Fc-Cε3/Cε4 region that interacts with 3-[3-(cholamidopropyl) dimethylammonio]-1-propane-sulfonate (CHAPS). Interaction sites 1 and 2 are the sites at which amino acids from FcεRIα and Fc-Cε3/Cε4 interact with each other. These sites

are described in more detail in the Examples and represent sites to target for drug design and mutein production.

One embodiment of the present invention is a model that represents a complex that includes a protein that binds to a Fc domain of an IgE antibody with an affinity that is at least equivalent to the affinity of the extracellular domain of human FcεRIα for any one of the following IgE antibodies: a human IgE antibody, a canine IgE antibody, a feline IgE antibody, an equine IgE antibody, a rat IgE antibody, and a murine IgE antibody. Such a model can represent an extracellular domain of a human FcεRIα protein, a canine FcεRIα protein, a feline FcεRIα protein, an equine FcεRIα protein, a murine FcεRIα protein, and a rat FcεRIα protein. Such a model can also represent a protein with altered substrate specificity, preferably designed based on a model of the present invention. WO 98/23964, *ibid.*, reports the ability of an isolated human FcεRIα protein to bind to canine, feline and equine IgE antibodies. Models of the present invention can be used to design a FcR with increased affinity for an antibody of a species other than self, such as, but not limited to, a human FcεRIα with increased affinity for a canine, feline or equine IgE antibody.

A model of the present invention can also represent a complex that includes a Fc domain of an antibody that binds to a FcεRIα protein with an affinity that is at least equivalent to the affinity of a human IgE antibody Fc-Cε3/Cε4 region for the extracellular domain of any of the following FcεRIα proteins: a human FcεRIα protein, a canine FcεRIα protein, a feline FcεRIα protein, an equine FcεRIα protein, a murine FcεRIα protein and a rat FcεRIα protein. Such a model can represent a FceRI-binding domain of

a human, canine, feline, equine, murine or rat Fc region. Such a model can also represent a Fc region with altered substrate specificity, preferably designed based on a model of the present invention.

The present invention includes a model that represents a complex between a FcR and a Fc domain that binds to an antibody or receptor of its respective class (i.e., IgE, IgG, IgM, IgA or IgD antibody class or corresponding Fc receptor). Also included is a model that represents a complex between a FcR and antibody designed to bind to an antibody or receptor, respectively, of a class other than the class to which the protein naturally binds. Such a model of the present invention can be produced, for example, by incorporating all or any part of the amino acid sequence of the other FcR or antibody into a 3-D model substantially representing the coordinates in Table 1. Such an embodiment includes any model that specifically incorporates any Ig domains that are placed in an orientation (packing interfaces and bend angles) that is based on the structure of the FcεRIα or a model that is based on the 1:1 stoichiometry predicted by the coordinates in Table 1. A preferred model of the present invention represents a complex including a FcR that binds to an IgE antibody or to an IgG antibody. In one embodiment, a model of the present invention is a 3-D model of a complex between an extracellular antibody binding domain of a FcR other than human FcεRIα, such as of a FcR that binds to an IgG antibody and an antibody. Such proteins and models thereof can be designed by homology modeling by, for example, altering the substrate specificity of a FcεRIα protein such that the altered protein binds an IgG antibody.

A preferred modified model of the present invention is a model that has a 3-D structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 10 angstrom when superimposed, using backbone atoms, on the 3-D model substantially represented by the atomic coordinates specified in Table 1. Preferably such a model has a 3-D structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 8 angstroms, preferably less than 7 angstroms, preferably less than 6 angstroms, preferably less than 5 angstroms, preferably less than 4 angstroms, preferably less than 3 angstroms, preferably less than 2 angstroms, and preferably less than 1 angstroms, when superimposed, using backbon3 atoms, on the 3-D model substantially represented by the atomic coordinates specified in Table 1. In this embodiment, such a model represents a FcR binding to an antibody. The backbone atoms are those atoms that form the backbone, or 3-D folding pattern, of the model. As such, backbone atoms are the base residues of amino acids, i.e., nitrogen, carbon, the alpha carbon and oxygen. Also preferred is a model modification that includes (a) a FcR protein having an amino acid sequence that shares at least about 30%, preferably at least about 40%, more preferably at least about 45%, more preferably at least about 50%, more preferably at least about 60% and even more preferably at least about 80% amino acid sequence homology, with a human FcεRIα protein, as determined using the program ALIGN with default parameters, optimal global alignment of two sequences with no short-cuts and (b) a Fc region having an amino acid sequence that shares at least about 30%, preferably at least about 40%, more preferably at least about 45%, more preferably at least about 50%, more preferably at least about 60% and even

more preferably at least about 80% amino acid sequence homology, with a Fc-Cε3/Cε4 region of a human IgE antibody, as determined using the program ALIGN with default parameters, optimal global alignment of two sequences with no short-cuts. It is to be noted that, using the same program and parameters, the extracellular domain of a human FcεRIα protein (i.e., soluble human FcεRIα protein) shares about 48% identity with feline and rat soluble FcεRIα proteins, about 49% with a murine soluble FcεRIα protein, about 50% identity with a canine soluble FcεRIα protein, and about 60% identity with an equine soluble FcεRIα protein. A preferred model of the present invention represents an IgE binding domain, i.e., a region that binds to an IgE antibody, complexed to a FcεRIα-binding domain, i.e., a region that binds to a FcεRIα protein.

One embodiment of the present invention is a 3-D model of a complex between a human FcεRIα protein and a human Fc-Cε3/Cε4 region produced by a method that includes the steps of: (a) crystallizing a complex between an extracellular domain of a human FcεRIα protein, such as, but not limited to a protein having amino acid sequence SEQ ID NO:2 or SEQ ID NO:4 and a human Fc-Cε3/Cε4 region, such as, but not limited to a protein having amino acid sequence SEQ ID NO:6; (b) collecting X-ray diffraction data from the crystallized complex; and (c) determining the model from the X-ray diffraction data, preferably in combination with an amino acid sequence of the proteins in the complex. A complex for crystal formation can be produced using a variety of techniques well known to those skilled in the art. As disclosed herein, human FcεRIα proteins and human Fc-Cε3/Cε4 region sto be crystallized are preferably produced in recombinant insect cells transformed with a gene encoding the respective proteins, such

as a baculovirus genetically engineered to produce the respective protein. The purity of the FcεRIα protein or Fc-Cε3/Cε4 region must be sufficient to permit the production of crystals that can be analyzed by X-ray crystallography to a resolution that permits determination of a 3-D model of the protein. Preferably the resolution is at least about 4.5 angstroms (i.e., 4.4 angstroms or better), more preferably at least about 4 angstroms, more preferably at least about 3.5 angstroms, more preferably at least about 3.25 angstroms, more preferably at least about 3 angstroms, more preferably at least about 2.5 angstroms, more preferably at least about 2 angstroms and even more preferably at least about 1.5 angstroms. Methods to obtain such purity levels are well known to those skilled in the art.

As disclosed herein, a preferred method to crystallize a complex between a FcεRIα protein and a Fc-Cε3/Cε4 region is by vapor distillation. Particularly preferred methods are disclosed in the Examples. It should be appreciated that the present invention also includes other methods known to those skilled in the art by which such a complex can be crystallized.

3-D models of some proteins have been determined; see, for example, Blundell et al., *Protein Crystallography*, Academic Press, London, 1976. However, as discussed herein, elucidation of the crystal structure of a complex between the extracellular domain of the human FcεRIα and a Fc-Cε3/Cε4 region of a human IgE was difficult. In one embodiment, crystal structure determination includes obtaining high-resolution data using synchrotron radiation. Such data can be collected, for example, at the Stanford Synchrotron Source Laboratory, Palo Alto, CA, or the Advanced Photon

Source at Argonne National Laboratories, Argonne, IL. Additional locations to collect such data include, but are not limited to, Brookhaven, NY, and Japan. In one embodiment, diffraction data from native and heavy-atom treated crystals provide an initial image of the protein structure which is refined into an electron density map. Details regarding data collection and interpretation are provided in the Examples section.

One embodiment of the present invention is a method to produce a 3-D model of a FcεRIα protein that includes positioning amino acid representations (i.e., representing amino acids) of the protein at substantially the coordinates listed in Table 1. That is, knowledge of the coordinates of the complex permits one skilled in the art to produce a model of the complex using those coordinates. Such a model, or any model which is essentially represented by a simple coordinate transformation of the coordinates specified in Table 1, can be represented in a variety of methods as heretofore disclosed and is included in the present invention.

In another embodiment, a model of the present invention can be refined to obtain an improved model, which is an example of a model modification, also referred to as a modified model. Refining methods can include, but are not limited to, further data collection and analysis; data collection from frozen crystals; introduction of solvent molecules to the structure; clarification of secondary structure; and analyses of crystallized complexes between a FcR and an antibody or inhibitory compound or of crystallized FcRs or antibodies alone. An additional model refinement method includes analyzing a 3-D model to predict amino acid residues that if replaced are likely to yield proteins with at least one improved function, effecting at least one such replacement,

determining whether the activity of the modified protein agrees with the prediction, and refining the model as necessary. Methods to determine whether the modification agrees with prediction include producing the modified protein and performing assays with that modified protein to determine if the protein does indeed exhibit the improved function(s), such as desired activity, stability and solubility properties. Assays to measure such functions are well known in the art; examples of several such assays are disclosed herein.

Another embodiment of the present invention is a modified 3-D model that represents a complex between a FcR other than a human FcεRIα protein represented by the 3-D model the coordinates of which are listed in Table 1 and an antibody other than human IgE as represented by the coordinates in Table 1. Preferably the amino acid sequence of the protein(s) to be modeled is known. In such a case, the modified model can be produced using the technique of homology modeling, preferably by incorporating (e.g., grafting, overlaying or replacing) all or any portion of the amino acid sequence of the other FcR or antibody into the 3-D model representing the coordinates of Table 1 to produce the modified model. General techniques for homology modeling, also referred to as molecular replacement, have been disclosed in, for example, Greer, 1990, *Proteins: Structure, Function, and Genetics 7*, 317-334; Havel et al., 1991, *J. Mol. Biol. 217*, 1-7; Schiffer et al., 1990, *Proteins: Structure, Function, and Genetics 8*, 30-43; and Lattman, 1985, *Methods Enzymol 115*, 55-77. However, such technology has not been applied to complexes between FcRs and antibodies since, until the present invention, no 3-D model of any FcR:antibody complex was available. Thus, the present invention now allows the

solving of the structures of a number of other natural and mutated forms of FcRs, antibodies or complexes thereof.

In one embodiment, a model of a FcR:Fc complex, such as, but not limited to a FcεRIα:Fc-Cε3/Cε4 complex, is produced by extracting the 3-D coordinates from a published figure or building a 3-D model with atoms from other domains wherein the domain 1 and 2 of the FcR and FcR-binding domains of the antibody are oriented as predicted for a complex between the human $FcεRIα_{1-176}$ protein and human $Fc\text{-}Cε3/Cε4_{222}$ protein. For example, a model of the present invention can be produced by orienting two known Ig domains into a bent confirmation similar to that of the two domains of the human FcεRIα protein. Such a model is referred to as a model in which domain 1 and domain 2 are oriented in a manner as specified by the structural coordinates listed in Table 1. This model can then be used in further molecular replacement methods. Such methods can include the steps of (a) orienting the model by three rotations; and (b) translating the model in one to three directions to produce additional model modifications.

Suitable FcRs or antibodies for which a 3-D model can be determined using homology modeling include any mammalian FcR or antibody, such as a protein that binds to IgE, IgG, IgM, IgA or IgD antibodies or an antibody that binds to the corresponding FcR. Preferred is a FcR protein that binds to an IgE antibody or an IgG antibody. Preferred FcRs that bind to IgE include human, canine, feline, equine, murine and rat FcεRIα proteins. Preferred antibodies that bind to FcRs include human, canine, feline,

equine, murine and rat antibodies. The present invention also includes the use of other Ig domains to produce models of the present invention.

One embodiment of the present invention is a 3-D model of a FcR:antibody complex in which one or both proteins have an improved function compared to an unmodified protein as well as a method to produce such a modified model. Such an improved function includes, but is not limited to, enhanced activity, enhanced stability and enhanced solubility. Such a modified model can be produced by replacing at least one amino acid based on information derived from analyzing the 3-D model representing the coordinates in Table 1, such that the replacement leads to a protein with an improved function. As used herein, a replacement refers to an (i.e., one or more) amino acid substitution, insertion, deletion, inversion and/or derivatization (e.g., acetylation, glycosylation, phosphorylation, PEG modification, biotinylation, and covalent attachment of other ligands or other compounds to the protein. In one embodiment, synthetic chemical methods are used to produce either a fragment or the entire protein to, for example, introduce non-natural amino acids or other chemical compounds into the structure of a FcR or antibody. For example, based on a structure of the present invention, one can design synthetic peptides or larger proteins that could be linked to produce an intact protein with IgE or FcR binding activity, the structure allowing one to design the start and stop points for these peptides, e.g., at surface accessible loops. In accordance with the present invention, an amino acid that is substituted or inserted can be a natural amino acid or an unnatural amino acid, including a derivitized amino acid.

Methods to identify regions in the protein that, if changed, yield a protein with an improved function are disclosed below.

The present invention includes use of a 3-D model of the present invention to identify a compound that inhibits binding between a FcR and an antibody. The advantages of using a 3-D model to identify inhibitory compounds are multi-fold in that the model depicts the site at which a Fc region of an antibody binds to its FcR, i.e., the antibody-binding domain, also referred to as the antibody binding site, and the FcR-binding domain, also referred to as the FcR binding site. The antibody binding site and the FcR binding site together form an FcR:antibody interaction site. As such, a large number of potential inhibitory compounds can be initially analyzed without having to perform *in vitro* or *in vivo* laboratory studies. As used herein, methods to identify inhibitory compounds include, but are not limited to, designing inhibitory compounds based on the 3-D model of a FcR, probing such a 3-D model with compounds that are potential inhibitors in order to identify those compounds that are actually inhibitory of the binding of an antibody to its FcR, screening a compound data base using such a 3-D model to identify compounds that inhibit such binding, and combinations thereof. Methods to use 3-D models to design, probe for, or screen for suitable inhibitory compounds are known to those skilled in the art. In particular, there are a number of computer programs that enable such methods. See, for example, PCT Publication No. WO 95/35367, by Wilson et al., published December 28, 1995, which is incorporated by reference herein in its entirety.

An inhibitory compound can be any natural or synthetic compound that inhibits the binding of an antibody to a FcR. Examples include, but are not limited to, inorganic compounds, oligonucleotides, proteins, peptides, antibodies, antibody fragments, mimetics of peptides or antibodies (such as, mimetics of antibody or receptor binding sites), and other organic compounds. Compounds can inhibit binding in either a competitive or non-competitive manner and can either interact at the binding site or allosterically. An inhibitory compound should be capable of physically and structurally associating with a FcR and/or an antibody such that the compound can inhibit binding between the two entitites. As such, an inhibitory compound is preferably small and is of a structure that effectively prevents or disrupts binding. Inhibitory compounds can be identified in one or multiple steps. For example, a compound initially identified that inhibits binding between an antibody and FcR to some extent can be used as a lead to design, probe or screen for a compound with improved characteristics, such as greater efficacy, safety, solubility, etc. A preferred inhibitory compound is a compound that is efficacious when administered to an animal in an amount that results in a serum concentration of from about 1 nanomolar (nM) to 100 micromolar (mM), with a concentration of from about 10 nM to 10 mM being more preferred.

One embodiment of the present invention is a method to identify a compound that inhibits the binding between an IgE antibody and a FcεRIα protein. Such a method includes the step of using a 3-D model substantially representing the atomic coordinates specified in Table 1 to identify such a compound. Included in the present invention are inhibitory compounds that interact directly with the IgE binding domain or the receptor

binding domain of the IgE antibody as well as compounds that interact indirectly with an FcεRIα protein, such as compounds that interact with the IgE binding domain, the FcεRIα binding domain, FcεRIα:Fc-Cε3/Cε4 interaction site 1, FcεRIα:Fc-Cε3/Cε4 interaction site 2, the hinge between domain Cε3 and domain Cε4 of the Fc-Cε3/Cε4 region, or a FcεRIα:Fc-Cε3/Cε4 region that interacts with CHAPS. In a preferred embodiment, an inhibitory compound interacts with at least one of the following regions of a model representing a FcεRIα:Fc-Cε3/Cε4 complex: a C strand of domain 2 of FcεRIα, a C'E loop of domain 2 of FcεRIα, a tryptophan-containing hydrophobic ridgeof FcεRIα, a linker between domain 1 and domain 2 of FcεRIα, a BC loop of domain 2 of FcεRIα, a FG loop of domain 2 of FcεRIα, a Cε2/Cε3 linker region of Fc-Cε3/Cε4, a BC loop of Fc-Cε3/Cε4, a DE loop of Fc-Cε3/Cε4, and a FG loop of Fc-Cε3/Cε4. Inhibitory compounds of the present invention preferably interact with at least one of the following amino acids: (a) a residue having a position in SEQ ID NO:2 selected from the group consisting of position 85, 86, 87, 110, 113, 117, 119, 126, 129, 130, 131, 132, 156, 157, and 158; (b) a residue having a position in SEQ ID NO:6 selected from the group consisting of position 4, 7, 8, 9, 10, 11, 37, 38, 39, 68, 69, 70, 99, 100, 101 and 102; and (c) a surface residue within about 10 angstroms of any of the residues listed in (a) or (b). Particularly preferred amino acids with which to interact are: (a) a residue within the FcεRIα pocket for the proline at position 101 of SEQ ID NO:6, such residues including, but not limited to positions 85, 86, 87 and 110 of SEQ ID NO:2; (b) a residue within the IgE pocket for the tyrosine at position 131 of SEQ ID NO:2, such residues including, but not limited to, positions 9, 11, 37, 39, and 99 of SEQ ID NO:6; and (c) a surface residue

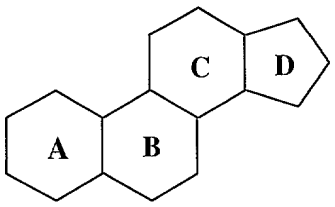
within about 10 angstroms of any of said residues of (a) or (b). It is to be noted that the ability to identify such key regions and residues is only possible in view of a model of the present invention. These regions and residues are a refinement of those identified using a FcεRIα model as described in 09/434,193, *ibid.* or WO 00/26246, *ibid.* In one embodiment, an inhibitory compound of the present invention is a peptide corresponding to at least a portion of any of the identified regions or a derivative thereof, such as a peptide mimetic or other compound that mimics that peptide.

One embodiment of a method to identify a compound that inhibits the binding between an IgE antibody and a FcεRIα protein includes the steps of: (a) generating a model substantially representing the atomic coordinates listed in Table 1 or of the binding domains thereof, on a computer screen; (b) generating the spacial structure of a compound to be tested; and (c) testing to determine if the compound interacts with said IgE binding domain or FcR binding domain, wherein such an interaction indicates that the compound is capable of inhibiting the binding of an IgE antibody to a FcεRIα protein. In a preferred embodiment, step (a) includes the step of identifying one or more amino acid(s) in the IgE binding domain of FcR binding domain of the model that interact directly with the corresponding domain. Preferably a compound to be tested will interact directly with one or more of those amino acid(s). Preferred amino acids with which an inhibitory compound should interact are disclosed herein.

The present invention also includes inhibitory compounds isolated in accordance with the methods disclosed herein. Methods to produce such compounds in quantities sufficient for use, for example, as protective agents (e.g., preventatives or therapeutics)

are known to those skilled in the art. It should also be appreciated that it is within the scope of the present invention to expand the use of models of the present invention to produce models of any suitable FcRs (i.e., model modifications) and to identify compounds that inhibit the binding of antibodies to such FcRs.

A preferred inhibitory compound of the present invention, or lead that can be used to produce a more efficacious inhibitory compound, is a saturated tetracyclic hydrocarbon perhydrocyclopentanophenanthrene or a derivative thereof. Such a compound can include a structure having the following formula:



It is to be understood that such a compound can have any number of "R" groups, even though they are not indicated in the formula. Examples of saturated tetracyclic hydrocarbon perhydrocyclopentanophenanthrenes include, but are not limited to, isoprenoids, terpenes, bile acids, detergents (such as CHAPS and CHAPSO) cholestanes, cholic acids, cholesterols, androgens, estrogens, and other steroids. A preferred inhibitory compound, or compound to use as a lead to design a more efficacious compound is 3-[3-(cholamidopropyl) dimethylammonio]-1-propane-sulfonate (CHAPS) or a compound having a similar ring structure. The interaction of CHAPS with amino acids in the FcεRIα protein and Fc-C3/C4 region is described in further detail in the Examples.

The present invention also includes use of a 3-D model of the present invention to rationally design and construct modified forms of FcRs or antibodies that have one or

more improved functions, such as, but not limited to, increased activity, increased stability and increased solubility compared to an unmodified FcR or antibody. Muteins of the present invention include full-length proteins as well as fragments (i.e., truncated versions) of such proteins.

One embodiment of the present invention is a FcR that comprises a mutein that binds to a Fc domain of an antibody. Such a mutein has an improved function compared to a protein comprising SEQ ID NO:2. Examples of such an improved function include, but are not limited to, increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility. Such a mutein can be produced by a method that includes the steps of: (a) analyzing a 3-D model substantially representing the atomic coordinates specified in Table 1 to identify at least one amino acid of the protein represented by the model which if replaced by a specified amino acid would effect the improved function of the protein; and (b) replacing the identified amino acid(s) to produce a mutein having the improved function. Knowledge of the coordinates allows one to target specific residues, e.g. in the hydrophobic core or on the surface, to generate an accessible set of variants that can then be selected for a particular property, e.g. high stability, high affinity, altered substrate specificity, or other desirable properties (i.e., improved functions). Without the coordinates, one would have to analyze an extraordinarily large number of variants, e.g., on the order of ~10^{11} possibilities. The structure, in contrast, allows one to pick the most relevant residues for selecting a desired property by, for example, phage display or other methods. In a preferred embodiment, replacement of one or more amino acids does not substantially disrupt the 3-D structure

of the protein; i.e., the modified protein, or mutein, is still capable of binding to the Fc domain of an antibody. A preferred mutein is a FcR that binds to a Fc domain of an IgE antibody, although the invention also covers muteins binding to other classes of antibodies.

In one embodiment, a mutein of the present invention has increased stability compared to its unmodified counterpart. As used herein, increased stability refers to the ability of a mutein to be more resistant, for example, to higher or lower temperature, to more acidic or basic pH, to higher or lower salt concentrations, to oxidation and/or reduction, to deamidation, to other forms of chemical degradation and to proteolytic degradation compared to unmodified FcR. Increased stability can also refer to the ability of a mutein of the present invention to be stable for a longer period of time either during storage (i.e., to have a longer shelf life) or during use (i.e., to have a longer half-life under reaction conditions) than does an unmodified protein. Muteins of the present invention can also exhibit a decreased entropy of unfolding, thereby stabilizing the proteins. Increased stability can be measured using a variety of methods known to those skilled in the art; examples include, but are not limited to, determination of melting temperature, thermal denaturation, pressure denaturation, enthalpy of unfolding, free energy of the protein, or stability in the presence of a chaotropic agents such as urea, guanidinium chloride, guanidinium thiocyanate, etc. A preferred mutein of the present invention has a melting temperature substantially higher than that of an unmodified FcR. Preferably the melting temperature of a mutein is at least about 1°C higher, and more preferably at least about 10°C higher than the melting temperature of the corresponding

unmodified protein. Also preferred is a mutein having binding activity over a pH range that is at least about 1 pH unit higher and/or lower than the active pH range of the corresponding unmodified protein.

Another embodiment of the present invention is a mutein that exhibits increased affinity for a Fc domain of an antibody compared to its unmodified counterpart. As used herein, a mutein having increased affinity is a FcR that exhibits a higher affinity constant (K_A) or lower dissociation constant (K_D) than its unmodified counterpart. Such a higher affinity constant can be achieved by increasing the association rate (k_a) between the mutein and the Fc domain and/or decreasing the dissociation rate (k_d) between the mutein and the Fc domain. A preferred mutein of the present invention has a K_A for a Fc domain of at least about 3×10^9 liters/mole (M^{-1}), which is equivalent to a K_D of less than or equal to about 3.3×10^{-10} moles/liter (M). More preferred is a mutein having a K_A for a Fc domain of at least about 2×10^{10} M^{-1}, and even more preferably of at least about 1×10^{11} M^{-1}. Also preferred is a mutein having a k_a for a Fc domain of at least about 1×10^5 liters/mole-second as well as a mutein having a k_d for a Fc domain of less than or equal to 3×10^{-5}/second. More preferred is a mutein having a k_a for a Fc domain of at least about 3×10^5 liters/mole-second, and even more preferably of 1×10^6 liters/mole-second. Also preferred are muteins having a k_d for a Fc domain of less than or equal to 1×10^{-5}/second or even more preferably less than or equal to 3×10^{-4}/second. A preferred Fc domain is that of an IgE antibody. Methods to measure such binding constants is well known to those skilled in the art; see, for example, Cook et al., 1997, *ibid.*, which reports the following values for the binding of human FcεRIα protein to human IgE: k_{a1} of 3.5 ($\pm$0.9)

x 10^5 $M^{-1}s^{-1}$; k_{a2} of 8.6 ($\pm$3.5) x 10^4 $M^{-1}s^{-1}$; k_{d1} of 1.2 ($\pm$0.1) x 10^{-2} s^{-1}; k_{d2} of 3.2 ($\pm$0.8) X 10^{-5} s^{-1}; K_{A1} of 2.0 X10^7 M^{-1}; K_{A2} of 2.9 X10^9 M^{-1}.

Another embodiment of the present invention is a mutein that exhibits altered substrate specificity compared to its unmodified counterpart. A mutein exhibiting altered substrate specificity is a mutein that binds with increased affinity to a Fc domain of an antibody class or antibody species of a different type than that normally bound by its unmodified counterpart. In one embodiment, a mutein of a human FcεRIα protein with altered substrate specificity is a FcR that binds with increased affinity to a IgE antibody of another mammal, such as, but not limited to, a canine, feline, equine, murine, or rat IgE antibody. In another embodiment, a mutein of a human FcεRIα protein with altered substrate specificity is a FcR that binds with increased affinity to an antibody of another class, such as IgG, IgM, IgA, or IgD, with IgG being preferred. Such a mutein can also show altered species substrate specificity. Methods to determine whether a mutein exhibits altered substrate specificity are well known to those skilled in the art.

Yet another embodiment of the present invention is a mutein that exhibits increased solubility compared to its unmodified counterpart. Such a protein is less likely to form aggregates. Methods to determine whether a mutein exhibits increased solubility are well known to those skilled in the art.

As disclosed herein, the 3-D model representing a FcεRIα:Fc-Cε3/Cε4 complex is advantageous in determining strategies for producing muteins having an improved function, e.g., for identifying targets to modify in order to obtain muteins having improved functions. Examples of targets are as follows. A key feature of the human

$Fc\varepsilon RI\alpha_{1-176}$ protein is the crystal contacts in five space groups, a subset of which are predicted to interact directly with a Fc domain of an IgE antibody. Such contacts are included in the IgE binding domain which is unique for human $Fc\varepsilon RI\alpha$ in that the domain includes a tryptophan-containing hydrophobic ridge positioned on the top face of the crystal structure (i.e., amino acids W87, W110, W113, and W156 of SEQ ID NO:2) and an FG loop comprising amino acids from 155 to 158 of SEQ ID NO:2 that protrudes above the interface in an unusual manner. Particularly preferred amino acids are residues at positions of 85, 86, 87, and 110 of SEQ ID NO:2. Another key feature is the interface between domain 1 and domain 2 (i.e., the D1D2 interface) which includes amino acids 12, 13, 14, 15, 16, 17, 18, 20, 84, 85 and 86 in D1 and 87, 88, 89, 90, 91, 92, 93, 95, 104, 106, 108, 110, 111, 161, 163, 164, and 165 in D2 of SEQ ID NO:2. Also important are the two domains themselves: D1 includes amino acids 1 through 86 of SEQ ID NO:2; and D2 includes amino acids 87 through 176 of SEQ ID NO:2. Another important feature is the cleft between D1 and D2, which can be identified using the coordinates. Other areas of interest include the hydrophobic core which can be identified using the coordinates, the A'B loop of D1, which includes amino acids 18 and 19, the EF loop of D1, which includes amino acids 59-63, the BC loop of D2, which includes amino acids 110-114, the C strand of D2, which includes amino acids 114-123, the CC' loop of D2, which includes amino acids 123-125, the C'E loop of D2, which includes amino acids 127-134, in the different confirmations observed in the five crystal forms, and the F strand of D2, which includes amino acids 147-155 of SEQ ID NO:2. Yet another striking feature is the finding that the amino and carboxyl termini of the human $Fc\varepsilon RI\alpha_{1-176}$ protein

are only 10 angstroms apart. Particularly preferred targets are a crystal contact cluster, a tryptophan-containing hydrophobic ridge, a FG loop in D2, a D1D2 interface, a cleft between D1 and D2, a domain 1, a domain 2, a hydrophobic core, a A'B loop of D1, a EF loop of D1, a BC loop of D2, a C strand of D2, a CC' loop of D2, a C'E loop of D2, a strand of D2, the amino terminal five residues of said protein, and the carboxyl terminal five residues of said protein, with FcεRIα:Fc-Cε3/Cε4 interaction site 1, a FcεRIα:Fc-Cε3/Cε4 interaction site 2, a C strand of domain 2 of FcεRIα, a C'E loop of domain 2 of FcεRIα, and a tryptophan-containing hydrophobic ridge of FcεRIα being particularly preferred. Preferred residues to target include residues at positions 85, 86, 87, 110, 113, 117, 119, 126, 129, 130, 131, 132, 156, 157 and 158 of SEQ ID NO:2. In one embodiment, preferred regions to target are listed in Tables 3, 4, and 5.

Table 3. Contact analysis between specified sets of atoms in FcεRIα:Fc-Cε3/Cε4 interaction site 1

```
================================================================================
set1= ( segid A )
set2= ( segid B )
definition of contact atoms: ( known and not hydrogen )
  maximum distance cutoff between contact atoms: 4.0

================================================================================

 List of contacting residue pairs between set1 and set2.  The atoms
 that form the closest contact between the particular pair of residues
 and the corresponding distance are listed.

   atom in set 1      atom in set 2      distance (A)

================================================================================
  [ LYS  117  NZ   ] [  GLY  335  O    ]    3.24203
  [ LYS  117  NZ   ] [  ASP  362  OD2  ]    3.40928
  [ ILE  119  CD1  ] [  ASN  394  O    ]    2.99234
  [ ALA  126  CB   ] [  ARG  393  O    ]    3.47281
  [ ALA  126  CB   ] [  ASN  394  C    ]    3.8627
  [ ALA  126  CB   ] [  GLY  395  N    ]    3.50267
  [ TYR  129  OH   ] [  ASP  362  O    ]    2.80047
  [ TYR  129  CE2  ] [  ALA  364  CB   ]    3.81077
  [ TRP  130  CZ2  ] [  ARG  334  NH2  ]    3.40032
  [ TRP  130  CZ3  ] [  HIS  424  CE1  ]    3.908
  [ TYR  131  CG   ] [  ARG  334  CG   ]    3.15693
  [ TYR  131  CE2  ] [  VAL  336  CG2  ]    3.33025
  [ TYR  131  CE2  ] [  ASP  362  O    ]    3.72658
  [ TYR  131  OH   ] [  ALA  364  N    ]    3.33849
  [ TYR  131  OH   ] [  HIS  424  ND1  ]    2.60229
  [ GLU  132  OE1  ] [  ARG  334  NH1  ]    2.4186
```

Table 4. Contact analysis between specified sets of atoms in FcεRIα:Fc-Cε3/Cε4 interaction site 2

```
================================================================================
set1= ( segid A )
set2= ( segid D )
definition of contact atoms: ( known and not hydrogen )
maximum distance cutoff between contact atoms: 4.0

================================================================================

 List of contacting residue pairs between set1 and set2.  The atoms
 that form the closest contact between the particular pair of residues
 and the corresponding distance are listed.

   atom in set 1      atom in set 2      distance (A)

================================================================================
  [ SER  85   OG   ] [  PRO  426  O    ]    3.61996
  [ SER  85   O    ] [  ARG  427  CG   ]    3.88945
  [ ASP  86   O    ] [  PRO  426  CB   ]    3.23037
  [ ASP  86   OD2  ] [  ARG  427  CD   ]    3.37831
  [ TRP  87   CH2  ] [  LEU  425  CD2  ]    3.4993
  [ TRP  87   CZ2  ] [  PRO  426  CD   ]    3.58257
  [ TRP  87   NE1  ] [  ARG  427  N    ]    3.96531
  [ TRP  110  CG   ] [  PRO  426  CG   ]    3.30731
  [ TRP  113  CH2  ] [  HIS  424  O    ]    3.3407
  [ TRP  156  CA   ] [  PRO  333  O    ]    3.71511
  [ TRP  156  O    ] [  ARG  334  CA   ]    3.63918
  [ TRP  156  O    ] [  GLY  335  N    ]    3.19027
  [ GLN  157  NE2  ] [  CYS  329  N    ]    3.96932
  [ GLN  157  NE2  ] [  ASN  332  ND2  ]    2.70954
  [ GLN  157  NE2  ] [  PRO  333  O    ]    3.96239
  [ GLN  157  OE1  ] [  ARG  334  NH1  ]    3.22424
  [ LEU  158  CD1  ] [  GLY  335  O    ]    3.71969
  [ LEU  158  CD1  ] [  VAL  336  O    ]    3.42542
  [ MAN  246  O2   ] [  ARG  427  NH2  ]    3.54884
```

Table 5. Contact analysis between specified sets of atoms in FcεRIα-CHAPs interaction

```
================================================================================
  set1= ( segid A )
  set2= ( segid E )
  definition of contact atoms: ( known and not hydrogen )
  maximum distance cutoff between contact atoms: 4.0

================================================================================

 List of contacting residue pairs between set1 and set2.  The atoms
 that form the closest contact between the particular pair of residues
 and the corresponding distance are listed.

   atom in set 1      atom in set 2      distance (A)

================================================================================
  [ ARG  111  NH1  ] [  CPS  101  O4   ]    3.46342
  [ TRP  113  NE1  ] [  CPS  101  O4   ]    3.2081
  [ TRP  113  CZ2  ] [  CPS  103  C16  ]    3.9932
  [ TYR  116  CB   ] [  CHA  102  O8   ]    3.23437
  [ LYS  117  CD   ] [  CHA  102  O6   ]    3.86424
  [ LYS  154  CD   ] [  CHA  102  O6   ]    3.11731
  [ TRP  156  CZ2  ] [  CPS  103  C11  ]    3.36681
  [ GLN  157  CG   ] [  CHA  102  O7   ]    3.90519
```

In accordance with the present invention, a mutein having an improved function can be produced by a method that includes replacing at least one amino acid based on information derived from analyzing a 3-D model of the present invention to produce the mutein having the improved function. Knowledge of the structure of the extracellular domain of a human FcεRIα protein crystal, for example, permits the rational design and construction of modified forms of the protein by permitting the prediction and production of substitutions, insertions, deletions, inversions and/or derivatizations that effect an improved function. That is, analysis of 3-D models of the present invention provide information as to which amino acid residues are important and, as such, which amino acids can be changed without harming the protein. In making amino acid replacements, it is preferred to use amino acid replacements that have similar numbers of atoms and that allow conservation of salt bridges, hydrophobic interactions and hydrogen bonds unless the goal is to purposefully change such interactions. The 3-D structure of the human

FcεRIα protein suggests that large deletions may not be desirable, particularly due to the relation between the various domains of the protein and the observation that most of the structure is well ordered in the crystal. An exception to this is the non-constrained loops of D1, which apparently could be deleted or shortened without harming the protein's function. These loops span amino acids 31-35 and 70-74 of SEQ ID NO:2.

It is to be appreciated that although one amino acid replacement capable of improving the function of a protein can substantially improve that function, more than one amino acid replacement can result in cumulative changes depending on the number and location of the replacements. For example, although one amino acid replacement capable of substantially increasing the stability of a protein can increase the melting temperature of that modified protein by about 1°C, about 5 to about 6 replacements may increase the melting temperature of the resultant protein by about 10°C.

In accordance with the present invention, the 3-D model of the complex has been analyzed, using techniques known to those skilled in the art, to determine the accessibility of the amino acids represented within the model to solvent. Such information is provided in, for example, Table 2.

A number of methods can be used to produce muteins of the present invention. One method includes the steps of: (a) analyzing a 3-D model substantially representing the coordinates specified in Table 1 to identify at least one amino acid of the modeled protein which if replaced by a specified amino acid would effect an improved function; and (b) replacing the identified amino acid(s) to produce a mutein having that improved function. In one embodiment, a method to produce a mutein includes the steps of (a)

comparing a key region of a model of a human FcεRIα protein with the amino acid sequence of a FcR having an improved function compared to the unmodified FcεRIα protein in order to identify at least one amino acid segment of the FcR with the improved function that if incorporated into the FcεRIα protein represented by the model would give the FcεRIα protein the improved function; and (b) incorporating the segment into the FcεRIα protein, thereby providing a mutein with the improved function. In another embodiment, a method to produce a protein includes the steps of: (a) using a model representing a human FcεRIα protein to identify a 3-D arrangement of residues that can be randomized by mutagenesis to allow the construction of a library of molecules from which a improved function can be selected; and (b) identifying at least one member of the mutagenized library having the improved function. In one example, a mutein is produced by a method that includes the steps of: (a) effecting random mutagenesis of nucleic acid molecules encoding a target of a FcεRIα protein as identified by analyzing a model of that protein, such as an IgE binding domain; (b) cloning such mutagenized nucleic acid molecules into a phage display library, wherein said phage display library expresses the target; and (c) identifying at least one member of the library that expresses a target with an improved function, such as an antibody binding domain exhibiting increased affinity for an antibody. As stated above, the model allows the use of this technique in a straightforward manner that could not be accomplished in the absence of the model. It is to be also noted that these methods can also be used with other models of the present invention to produce muteins of the present invention.

The present invention includes a number of methods, based on analysis of a 3-D

model of the present invention, to replace (i.e., add, delete, substitute, invert, derivatize) at least one amino acid residue in the protein represented by the model in order to produce a mutein of the present invention. Such methods include, but are not limited to: (a) replacing at least one amino acid in at least one non-constrained loop of domain 1 in an area proximal to the FceRI gamma chain putative binding site; (b) joining an amino-terminal amino acid residue to a carboxyl-terminal amino acid residue of an extracellular domain of a FcεRIα protein; (c) replacing at least one amino acid site with an amino acid suitable for derivatization; (d) replacing at least one pair of amino acids of the protein with a cysteine pair to enable the formation of a disulfide bond that stabilizes the protein; (e) removing at least a portion of the region between the B strand and C strand of domain 1; (f) removing at least a portion of the region between the C strand and E strand of domain 1; (g) replacing at least one amino acid in the IgE binding domain in order to increase the affinity between an IgE antibody and the protein; (h) replacing at least one amino acid of the protein with an amino acid such that the replacement decreases the entropy of unfolding of the protein; (i) replacing at least one asparagine or glutamine of the protein with an amino acid that is less susceptible to deamidation than is the amino acid to be replaced; (j) replacing at least one methionine, histidine or tryptophan with an amino acid that is less susceptible to an oxidation or reduction reaction than is the amino acid to be replaced; (k) replacing at least one arginine of the protein with an amino acid that is less susceptible to dicarbonyl compound modification than is the amino acid to be replaced; (l) replacing at least one amino acid of the protein susceptible to reaction with a reducing sugar sufficient to reduce protein function with an amino acid less susceptible

to that reaction; (m) replacing at least one amino acid of the protein with an amino acid capable of increasing the stability of the inner core of the protein; (n) replacing at least one amino acid of the protein with at least one N-linked glycosylation site; (o) replacing at least one N-linked glycosylation site of the protein with at least one amino acid that does not comprise an N-linked glycosylation site; and (p) replacing at least one amino acid of the protein with an amino acid that reduces aggregation of the protein.

Amino acid replacements can be carried out using recombinant DNA techniques known to those skilled in the art, including site-directed mutagenesis (e.g., oligonucleotide mutagenesis, random mutagenesis, polymerase chain reaction (PCR)-aided mutagenesis, gapped-circle site-directed mutagenesis) or chemical synthetic methods of a nucleic acid molecule encoding the desired protein, such as, but not limited to a human FcεRIα protein, followed by expression of the mutated gene in a suitable expression system, preferably an insect, mammalian, bacterial, yeast, insect, or mammalian expression system. See, for example, Sambrook et al., *ibid.*

One embodiment of the present invention is a mutein in which at least one amino acid in at least one non-constrained loop of a FcεRIα protein is replaced in order to improve a function of the protein. Finding that the human FcεRIα protein had such loops was surprising, and it is believed, without being bound by theory, that a mutein in which at least a portion of at least one such loop is replaced, would at least exhibit enhanced stability. In a preferred embodiment, at least a portion of one or more of such loops is (are) deleted. Preferred loops to replace are in domain 1 (i.e., spanning amino acids 31-35 and 70-74 of SEQ ID NO:2), preferably in an area proximal to the FceRI gamma

chain putative binding site, i.e., the site on the FcεRIα protein to which the gamma chain of the high affinity Fc epsilon receptor is thought to bind. In a preferred embodiment, one or more amino acids is replaced to make loops shorter, but including 1 or 2 hydrophobic residues to pack toward the protein interior and at least one hydrophilic residue to maintain solubility.

Another embodiment of the present invention is a mutein of the extracellular domain of a FcεRIα protein in which an N-terminal (amino-terminal) amino acid residue is joined, preferably covalently, to a C-terminal (carboxyl-terminal) amino acid residue in order to improve a function of the protein. Finding that the N-termini and C-termini of the human FcεRIα protein were only 10 angstroms apart was quite surprising. Without being bound by theory, it is believed that such a mutein would at least exhibit enhanced stability. Furthermore, a covalent linker used to join the termini could also include a substance useful, for example, to anchor a mutein on a surface, as would be useful, for example, in a diagnostic assay, or to label the mutein. For a protein consisting of SEQ ID NO:2, a preferred N-terminal residue is an amino acid residue at position 1, 2, or 3 of SEQ ID NO:2, and a preferred C-terminal residue is an amino acid residue at position 174, 175, or 176 of SEQ ID NO:2. Covalent linkage can be accomplished by methods known to those skilled in the art, such as, but not limited to, adding one or more N-terminal and C-terminal cysteines and crosslinking them with chemical compounds, adding additional residues in the coding sequence to allow the formation of a disulfide bond, or adding one or more lysines and coupling them through a 10 angstrom linker, and including non-natural amino acid analogues by synthetic methods or by a combination of

biosynthetic and organosynthetic methods. Examples of a substance to add to a covalent linker includes: ligands useful in allowing for the attachment of a mutein to a surface, such as biotin and related compounds, avidin and related compounds, metal binding compounds, sugar binding compounds, immunoglobulin binding domains, and other tag domains; and detectable markers, such as enzyme labels, physical labels, radioactive labels, fluorescent labels, chemiluminescent labels, and chromophoric labels. Examples include, but are not limited to, alkaline phosphatase, horseradish peroxidase, digoxygenin, luciferase, other light-generating enzymes and magnetic beads. It is also to be noted that ligands can function as detectable markers.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid suitable for derivatization. Muteins in which at least one amino acid is replaced with an amino acid suitable for derivatization include proteins that are chemically modified (e.g., a lysine already existing on the protein is modified) as well as those in which an amino acid residue is replaced with a different amino acid residue (e.g., a glycine with a lysine) as well as proteins to which a substance is added, preferably to the amino or carboxyl terminus of the protein. Examples of such substances include ligands and detectable markers as disclosed above. Preferable amino acids to replace include residues that are solvent exposed (e.g., those listed in Table 2), but that are preferably not within about 10 angstroms of the IgE binding domain. In one embodiment, a glycosylation site, or other solvent exposed site, is replaced with a charged or polar residue to increase solubility or create more stable muteins. Glycosylation sites in human FcεRIα protein include amino acids 21, 42, 50 74, 135, 140,

and 166 of SEQ ID NO:2. A preferred amino acid to use as a replacement, or to chemically modify directly, includes a cysteine or a lysine, with a cysteine being preferred. Compounds to use in chemical derivatizations are known to those skilled in the art; cysteines can, for example, be derivatized with maleimides.

Another embodiment of the present invention is a mutein in which a pair of amino acids have been replaced with a cysteine pair in order to improve the function of the mutein, at least by increasing stability. Cysteine pairs can be substituted into a FcεRIα protein at any two residue positions identified with available programs and algorithms that would allow the formation of an undistorted disulfide bridge. In one embodiment, a serine and lysine near the termini of the protein is each replaced with a cysteine. In another embodiment, cysteine pairs are replaced with other amino acids, such as serines to eliminate non-essential disulfide bonds.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced in the region between the B strand and C strand of domain 1 and/or the region between the C and E strand of domain 1. In a preferred embodiment, at least a portion of such a region is deleted.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced in the IgE binding domain in order to increase the affinity between an IgE antibody and the protein. Preferred residues to replace are in or near the IgE binding domain, or IgE binding site, as determined by analysis of the 3-D model. Such residues are preferably within about 10 angstroms of residues identified by mutagenesis and further shown by model to be in an IgE binding site. Examples of such residues

include amino acids 87, 110, 113, 115, 117, 118, 120, 121, 122, 123, 128, 129, 131, 149, 153, 154, 155, 156, 157, 158, and 159 of SEQ ID NO:2, and amino acids within 10 angstroms of such listed amino acids. In one embodiment, preferred amino acids to replace include amino acids 87, 115, 117, 118, 120-123, 128, 129, 131, 149, 153, 155 and 159 of SEQ ID NO:2 as well as any surface residue within about 10 angstroms of any of the listed amino acids, with amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 or SEQ ID NO:4 as well as any surface residue within about 10 angstroms of amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 being particularly preferred. It is to be noted that amino acids 115, 118, 120, 131, 149 and 155 of SEQ ID NO:2 are buried, and that amino acids that are partially buried or glycine include residues 122, 129 and 153. Additional amino acid residues to target include those in the A'B loop of D1, and EF loop of D1. Note that these residues are not the same as those shown in mutation studies to affect IgE binding since some of those mutants have mutations in amino acids that are internal to the protein; this finding can only be made by analysis of a model of the present invention.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid capable of increasing the stability of the inner core or surface of the protein. Preferred amino acids to replace are hydrophilic residues located in the hydrophobic core of the protein and/or hydrophobic amino acids at the protein surface that are not within about 10 angstroms of the IgE binding domain residues of D1 or D2. Preferred amino acids to replace into the hydrophobic core are hydrophobic residues such as, but not limited to, tryptophan, leucine, isoleucine, valine and alanine, as

well as space filling amino acids, such as other aromatic amino acids. Preferred amino acids to replace onto the surface are polar amino acids, such as, but not limited to, glutamic acid, glutamine, aspartic acid, asparagine, histidine and serine. Muteins having one or more such amino acid replacements would exhibit at least increased stability and/or reduced aggregation. Additional preferred amino acid replacements are those that introduce salt bridges at the protein surface to stabilize protein folds. It is noted that the cysteines at positions 26 and 68 of SEQ ID NO:2 form a disulfide bond in domain 1 that is somewhat exposed to solvent, depending especially on the conformation of the D1 "30 loop" (i.e., amino acids 31-35 of SEQ ID NO:2). In one embodiment, changes in neighboring residues can be made in, for example, residues 1-5, 27-37, 49-52, or 69-75, to bury this disulfide from exposure to solvent. For example, phage display of receptors with randomized mutations in the 30 loop, might be useful for selecting receptors that react less well with reducing reagents and have a more stable D1 core.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid that decreases the entropy of unfolding of the protein. The entropy of unfolding of a protein can be measured and compared to that of another protein using techniques known to those skilled in the art. A number of methods known to those skilled in the art can be used to reduce the number of protein conformations possible in the unfolded state, thereby improving the ability of the protein to fold correctly. One embodiment of the present invention for decreasing the entropy of unfolding includes replacing at least one amino acid of the protein with a specified amino acid in order to maintain certain desirable phi and psi backbone conformation angles in

the protein; see, for example, PCT International Publication No. WO 89/01520, by Drummond et al., published February 23, 1989. For example, a proline residue in a protein constrains the backbone conformation to certain restricted angles. Analysis of a 3-D model of a protein of the present invention permits the identification of candidate replacement positions in the protein that have the conformation expected for a proline, but that do not have a proline in them. Such knowledge is used to introduce prolines into such candidate replacement positions to "anchor" the resultant mutein in the desired conformation. The 3-D model also permits the identification of candidate replacement sites that if replaced with a proline do not substantially disrupt the 3-D structure of the resultant protein. Similarly, glycines in appropriate positions can be replaced with an amino acid having a β carbon atom or a branched β carbon atom, preferably an alanine, in order to stabilize the backbone of the protein.

Another embodiment of the present invention is a mutein in which at least one asparagine or glutamine is replaced with an amino acid that is less susceptible to deamidation. Preferred amino acids to replace include solvent accessible asparagines and glutamines.

Another embodiment of the present invention is a mutein in which at least one methionine, histidine or tryptophan is replaced with an amino acid that is less susceptible to an oxidation or reduction reaction. Preferred amino acids to replace include M98, H70, and H41. It would not be preferred to replace any of the tryptophans, nor H108 or H134 of SEQ ID NO:2.

Another embodiment of the present invention is a mutein in which at least one arginine is replaced with an amino acid that is less susceptible to dicarbonyl compound modification. Although R174 could be changed, it would probably not be preferable to change amino acids at the D1D2 interface or near the IgE binding site, such as amino acids 15, 106, or 111 of SEQ ID NO:2.

Another embodiment of the present invention is a mutein in which at least one amino acid that is susceptible to reaction with a reducing sugar sufficient to reduce protein function is replaced with an amino acid that is less susceptible to such a reaction. For example, lysines, glutamines and asparagines that could react with a sugar, such as galactose, glucose or lactose can be replaced with non-reactive amino acids.

Another embodiment of the present invention is a mutein in which one or more N-linked glycosylation sites are added to or removed from the protein, preferably by substitution with an appropriate amino acid. A FcεRIα protein with additional N-linked glycosylation sites is more soluble. The ability to design a FcεRIα protein having fewer, or no, N-linked glycosylation sites is also valuable as production of such a protein from production run to production run is likely to be more uniform. One embodiment is a FcεRIα mutein with no N-linked glycosylation sites that is stable, active, and soluble. Such a protein has an advantage of being produced in *E.* coli at low cost. In one embodiment, one or more exposed hydrophobic amino acids are changed to charged residues that form salt bridges to stabilize the protein fold and make it soluble. It is to be noted that the glycosylation sites that appear to be most often observed in the different crystal structures in the same conformation are the carbohydrate attached to positions 42

and 166 of SEQ ID NO:2. The carbohydrate attached to position 42 always appears to cover the phenylalanine at position 60 of SEQ ID NO:2. As such, one embodiment of the present invention is to remove the glycosylation site at position 42, e.g., by substitution with a suitable amino acid. This embodiment has the additional advantage that the resultant mutein has an exposed phenylalanine at position 60, thereby leading to increased IgE binding activity.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid that reduces aggregation and increases solubility of the protein, such as, for example, replacing one or more hydrophobic residues on the surface with one or more hydrophilic residues. Other examples of such amino acids to replace are disclosed herein.

Another embodiment of the present invention to enhance stability is the addition of polyethylene glycol (PEG) groups to a FcR protein, i.e., to produce a "pegylated" FcR protein. In one embodiment, the PEG group(s) can substitute for carbohydrate group(s) due to removal of one or more N-glycosylation sites. Such PEG group(s) can be attached to easily modifiable residues, such as cysteines or lysines, on the surface of the protein, such residues identifiable by analysis of a 3-D model of the present invention.

Another embodiment of the present invention is a mutein that comprises a FcR having a substance, such as a ligand or detectable marker, attached to an amino acid of the protein such that the substance does not substantially interfere with the antibody binding activity of the protein. The substance is attached in such a manner that the substance is also capable of performing its function, such as binding to a second member

of a ligand pair or enabling detection of the protein. The FcR to which a substance is attached can be either an unmodified protein or a mutein of the present invention. Suitable attachment sites can be identified using 3-D models of the present invention. Preferred attachment sites include solvent exposed amino acids, such as those listed in Table 2. Substances can be attached, or conjugated, to the protein using techniques known to those skilled in the art. It is to be appreciated that a preferred method to attach a substance to an amino acid is to modify that amino acid to have a reactive attachment site, such as is present on cysteine and lysine amino acids. As such, an attachment site comprising a solvent exposed amino acid refers to the nature of the amino acid prior to any modification required for attachment. Examples of suitable substances to attach to a FcR include any compound capable of binding to or reacting with another substance, such as those described for attachment to a covalent linker.

It is to be appreciated that muteins of the present invention can include amino acids which are not modified because they would negatively impact the function of the protein. Such amino acids can be identified using a 3-D model of the present invention.

It should also be appreciated that it is within the scope of the present invention to expand the use of models of the present invention to produce models of and make modifications to any suitable FcRs or other Ig domain-containing proteins to produce muteins having a desired function.

The present invention also includes a mutein that binds to an IgE binding domain of a FcεRIα protein, wherein the mutein has an improved function compared to a Fc-Cε3/Cε4 protein comprising amino acid sequence SEQ ID NO:6. Such an improved

function can include increased stability compared to the stability of a human IgE Fc region comprising amino acid sequence SEQ ID NO:6, increased affinity for a FcεRIα protein compared to the FcεRIα affinity of a human IgE Fc region comprising amino acid sequence SEQ ID NO:6, altered substrate affinity compared to the affinity for human FcεRIα of a human IgE Fc region comprising amino acid sequence SEQ ID NO:6, and increased solubility compared to the solubility of a human IgE Fc region comprising amino acid sequence SEQ ID NO:6. Such a mutein is produced by a method that includes the steps of (a) analyzing a three-dimensional model substantially representing the atomic coordinates specified in Table 1 to identify at least one amino acid of the Fc-Cε3/Cε4 protein represented by said model which if replaced by a specified amino acid would effect said improved function of said Fc-Cε3/Cε4 protein; and (b) replacing said identified amino acid(s) to produce said mutein having said improved function. Fc muteins can be identified and produced in a manner similar to that described herein for FcR muteins. Antibody muteins have a variety of uses, including but not limited to, diagnostic and therapeutic uses. For example, muteins could be used to image cells that express an antibody receptor protein, such as NMR-specific labeling for *in vivo* imaging to detect, for example, mast cell cancers, asthma, and other pathologies, or to treat cancers that express an antibody receptor protein using, for example, radioimmune therapy of derivatized IgE. Muteins could also be used for monitoring FcR expression in atopic individuals (e.g. with a tag for one-step FACS analysis) or for monitoring IgE in atopic individuals. Muteins could also be used as inhibitors or as toxin-IgE-Fc fusion proteins to target FcR-expressing cells to kill them (e.g. in mast cell tumors or severe

allergy). Also muteins that affect the low affinity affinity IgE-receptor (FceRII) binding but not FceRI binding could be designed or selected.

The present invention also includes nucleic acid molecules that encode muteins of the present invention as well as recombinant molecules and recombinant cells that include such nucleic acid molecules. Methods to produce such proteins are also disclosed herein.

The present invention also includes the following novel structures as identified by a 3-D model of the present invention. Preferred structures exhibiting direct interaction between IgE and FcεRIα include FcεRIα:Fc-Cε3/Cε4 interaction site 1, a FcεRIα:Fc-Cε3/Cε4 interaction site 2, a C strand of domain 2 of FcεRIα, a C'E loop of domain 2 of FcεRIα, and a tryptophan-containing hydrophobic ridge of FcεRIα. Other preferred structures include a crystal contact cluster involved in IgE binding; a FG loop in D2; a D1D2 interface; a cleft between D1 and D2; a domain 1; a domain 2; a hydrophobic core; a A'B loop of D1; a EF loop of D1; a BC loop of D2; a CC' loop of D2; and a strand of D2. Particularly preferred are (a) a FcεRIα:Fc-Cε3/Cε4 interaction site 1 pocket comprising an amino acid residue at position 131 of SEQ ID NO:2 and amino acid residues at positions 9, 11, 37, 39, and 99 of SEQ ID NO:6 and (b) a FcεRIα:Fc-Cε3/Cε4 interaction site 2 pocket comprising amino acid residues at positions 85, 86, 87, and 110 of SEQ ID NO:2 and amino acid residue at position 101 of SEQ ID NO:6. Also included herein are nucleic acid molecules to encode such structures as well as recombinant molecules and recombinant cells that include such nucleic acid molecules. Also included are methods to produce such structures and models thereof.

The present invention also includes isolated nucleic acid molecules encoding proteins of the present invention, including, but not limited to, unmodified proteins, novel structures within such proteins, and muteins. As used herein, an isolated nucleic acid molecule encoding a protein is a nucleic acid molecule that has been removed from its natural milieu. As such, "isolated" does not reflect the extent to which the nucleic acid molecule has been purified. An isolated nucleic acid molecule can be DNA, RNA, or derivatives of either DNA or RNA.

A nucleic acid molecule encoding a mutein of the present invention can be produced by mutation of parental protein genes (e.g., unmodified or previously modified protein-encoding genes, or portions thereof) using recombinant DNA techniques heretofore disclosed or by chemical synthesis. Resultant mutein nucleic acid molecules can be amplified using recombinant DNA techniques known to those skilled in the art, such as PCR amplification or cloning (see, for example, Sambrook et al., *ibid.*), or by chemical synthesis. A mutein can also be produced by chemical modification of a protein expressed by a nucleic acid molecule encoding an unmodified protein or mutein-encoding gene.

Proteins of the present invention can be produced in a variety of ways, including production and recovery of recombinant proteins and chemical synthesis. In one embodiment, a protein of the present invention is produced by culturing a cell capable of expressing the protein under conditions effective to produce the protein, and recovering the protein. A preferred cell to culture is a recombinant cell that is capable of expressing the protein, the recombinant cell being produced by transforming a host cell with one or

more nucleic acid molecules of the present invention. Transformation of a nucleic acid molecule into a host cell can be accomplished by any method by which a nucleic acid molecule can be inserted into a cell. Transformation techniques include, but are not limited to, transfection, electroporation, microinjection, lipofection, adsorption, and protoplast fusion. A recombinant cell may remain unicellular or may grow into a tissue, organ or a multicellular organism. Transformed nucleic acid molecules of the present invention can remain extrachromosomal or can integrate into one or more sites within a chromosome of a host cell in such a manner that their ability to be expressed is retained.

Suitable host cells to transform include any cell that can be transformed. Host cells can be either untransformed cells or cells that are already transformed with at least one nucleic acid molecule. Host cells of the present invention can be endogenously (i.e., naturally) capable of producing a protein of the present invention, but such cells are not preferred. Host cells of the present invention can be any cell that when transformed with a nucleic acid molecule of the present invention are capable of producing a protein of the present invention, including bacterial, yeast, other fungal, insect, animal, and plant cells. Preferred host cells include bacterial, yeast, insect and mammalian cells, and more preferred host cells include *Escherichia*, *Bacillus*, *Saccharomyces, Pichia*, *Trichoplusia*, *Spodoptera* and mammalian cells. Particularly preferred host cells are *Trichoplusia ni* cells and *Spodoptera frugiperda* cells with *T. ni* cells being particularly preferred.

A recombinant cell is preferably produced by transforming a host cell with a recombinant molecule comprising a nucleic acid molecule of the present invention operatively linked to an expression vector containing one or more transcription control

sequences. The phrase operatively linked refers to insertion of a nucleic acid molecule into an expression vector in a manner such that the molecule is able to be expressed when transformed into a host cell. As used herein, an expression vector is a DNA or RNA vector that is capable of transforming a host cell, of replicating within the host cell, and of effecting expression of a specified nucleic acid molecule. Expression vectors can be either prokaryotic or eukaryotic, and are typically viruses or plasmids. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including in bacterial, yeast, other fungal, insect, animal, and plant cells. Preferred expression vectors of the present invention can direct gene expression in bacterial, yeast, insect and mammalian cells.

Nucleic acid molecules of the present invention can be operatively linked to expression vectors containing regulatory control sequences such as promoters, operators, repressors, enhancers, termination sequences, origins of replication, and other regulatory control sequences that are compatible with the host cell and that control the expression of the nucleic acid molecules. In particular, recombinant molecules of the present invention include transcription control sequences. Transcription control sequences are sequences which control the initiation, elongation, and termination of transcription. Particularly important transcription control sequences are those which control transcription initiation, such as promoter, enhancer, operator and repressor sequences. Suitable transcription control sequences include any transcription control sequence that can function in at least one of the recombinant cells of the present invention. A variety of such transcription

control sequences are known to those skilled in the art. Preferred transcription control sequences include those which function in bacterial, yeast, insect and mammalian cells.

It may be appreciated by one skilled in the art that use of recombinant DNA technologies can improve expression of transformed nucleic acid molecules by manipulating, for example, the number of copies of the nucleic acid molecules within a host cell, the efficiency with which those nucleic acid molecules are transcribed, the efficiency with which the resultant transcripts are translated, and the efficiency of post-translational modifications. Recombinant techniques useful for increasing the expression of nucleic acid molecules of the present invention include, but are not limited to, operatively linking nucleic acid molecules to high-copy number plasmids, integration of the nucleic acid molecules into one or more host cell chromosomes, addition of vector stability sequences to plasmids, substitutions or modifications of transcription control signals (e.g., promoters, operators, enhancers), substitutions or modifications of translational control signals (e.g., ribosome binding sites, Shine-Dalgarno sequences), modification of nucleic acid molecules of the present invention to correspond to the codon usage of the host cell, deletion of sequences that destabilize transcripts, and use of control signals that temporally separate recombinant cell growth from recombinant protein production during fermentation. The activity of an expressed recombinant protein of the present invention may be improved by fragmenting, modifying, or derivatizing nucleic acid molecules encoding such a protein.

In accordance with the present invention, recombinant cells can be used to produce proteins by culturing such cells under conditions effective to produce such a

protein, and recovering the protein. Effective conditions to produce a protein include, but are not limited to, appropriate media, bioreactor, temperature, pH and oxygen conditions that permit protein production. An appropriate medium refers to any medium in which a cell of the present invention, when cultured, is capable of producing the protein. An effective medium is typically an aqueous medium comprising assimilable carbohydrate, nitrogen and phosphate sources, as well as appropriate salts, minerals, metals and other nutrients, such as vitamins. The medium may comprise complex nutrients or may be a defined minimal medium. Cells of the present invention can be cultured in conventional fermentation bioreactors, which include, but are not limited to, batch, fed-batch, cell recycle, and continuous fermentors. Culturing can also be conducted in shake flasks, test tubes, microtiter dishes, and petri plates. Culturing is carried out at a temperature, pH and oxygen content appropriate for the recombinant cell. Such culturing conditions are well within the expertise of one of ordinary skill in the art.

Depending on the vector and host system used for production, resultant proteins may either remain within the recombinant cell; be secreted into the fermentation medium; be secreted into a space between two cellular membranes, such as the periplasmic space in *E. coli*; or be retained on the outer surface of a cell or viral membrane. The phrase "recovering the protein" refers simply to collecting the whole fermentation medium containing the protein and need not imply additional steps of separation or purification. Proteins of the present invention can be purified using a variety of standard protein purification techniques, such as, but not limited to, affinity chromatography, ion exchange chromatography, filtration, electrophoresis, hydrophobic interaction chromatography, gel

filtration chromatography, reverse phase chromatography, chromatofocusing and differential solubilization.

The present invention also includes isolated (i.e., removed from their natural milieu) antibodies that selectively bind to a FcR or antibody of the present invention. As used herein, the term "selectively binds to" refers to the ability of antibodies of the present invention to preferentially bind to specified proteins of the present invention. Binding can be measured using a variety of methods standard in the art including enzyme immunoassays (e.g., ELISA), immunoblot assays, etc.; see, for example, Sambrook et al., *ibid.* Isolated antibodies of the present invention can include antibodies in a bodily fluid (such as, but not limited to, serum), or antibodies that have been purified to varying degrees. Antibodies of the present invention can be polyclonal or monoclonal. Functional equivalents of such antibodies, such as antibody fragments and genetically-engineered antibodies (including single chain antibodies or chimeric antibodies that can bind to more than one epitope) are also included in the present invention. Antibodies can be produced using methods known to those skilled in the art. A preferred method to produce antibodies of the present invention includes (a) administering to an animal an effective amount of a protein of the present invention to produce the antibodies and (b) recovering the antibodies. In another method, antibodies of the present invention are produced recombinantly using techniques as heretofore disclosed to produce proteins of the present invention. Antibodies raised against defined proteins can be advantageous because such antibodies are not substantially contaminated with antibodies against other

substances that might otherwise cause interference in a diagnostic assay or side effects if used in a therapeutic composition.

Antibodies of the present invention have a variety of potential uses that are within the scope of the present invention. Examples of such uses are disclosed in WO 98/27208, *ibid.*, see, for example, page 24; such uses are incorporated by reference herein in their entireties.

A FcR of the present invention can include chimeric molecules comprising at least a portion of a FcR that binds to an antibody and a second molecule that enables the chimeric molecule to be bound to a substrate in such a manner that the antibody receptor portion binds to the antibody in at least as effective a manner as a FcR that is not bound to a substrate. An example of a suitable second molecule includes a portion of an immunoglobulin molecule or another ligand that has a suitable binding partner that can be immobilized on a substrate, e.g., biotin and avidin, or a metal-binding protein and a metal (e.g., His), or a sugar-binding protein and a sugar (e.g., maltose). An antibody of the present invention can also be part of a chimeric molecule.

The present invention includes uses of proteins, antibodies and inhibitory compounds of the present invention for the diagnosis and treatment of allergy and the regulation of other immune responses in an animal.

One embodiment is a therapeutic composition comprising at least one of the following therapeutic compounds: an inhibitory compound of the present invention, a mutein of the present invention, or an antibody of the present invention. Also included is a method to protect an animal from allergy or other abnormal immune responses. Such a

method includes the step of administering a therapeutic composition of the present invention to the animal. As used herein, the ability of a therapeutic composition of the present invention to protect an animal from allergy or other abnormal immune responses refers to the ability of that composition to, for example, treat, ameliorate or prevent allergy or other abnormal immune responses. General characteristics of therapeutic compositions and methods to produce and use such therapeutic compositions are disclosed, for example, in WO 98/27208, *ibid.*, see, for example, page 39-47; such compositions and methods are incorporated by reference herein in their entireties. It is to be noted that although the compositions and methods disclosed in WO 98/27208, *ibid.*, relate to feline FcεRIα proteins, they are also applicable to therapeutic compositions of the present invention. Therapeutic compositions of the present invention are advantageous because they can be derived from analysis of 3-D models of the present invention and have improved functions, such as efficacy and safety.

Another embodiment is a diagnostic reagent comprising a mutein of the present invention. As used herein, a diagnostic reagent is a composition that includes a mutein that is used to detect allergy or other abnormal immune responses in an animal. Also included in the present invention are methods, including *in vivo* methods and *in vitro* methods, to (a) detect allergy or other abnormal immune response, or susceptibility thereto, in an animal, comprising use of a diagnostic reagent comprising a mutein of the present invention and (b) to enhance the performance of an IgE binding assay, said method comprising incorporating into the assay a mutein of the present invention. General characteristics of diagnostic reagents and methods to produce and use such

diagnostic reagents are disclosed, for example, in WO 98/27208, *ibid.*, see, for example, page 2-39; such reagents and methods are incorporated by reference herein in their entireties. It is to be noted that although the reagents and methods disclosed in WO 98/27208, *ibid.*, relate to feline FcεRIα proteins, they are also applicable to diagnostic reagents, kits and detection methods of the present invention. Muteins of the present invention are advantageous in such applications because of their enhanced affinity for antibodies, altered specificity, enhanced solubility and/or enhanced stability, enabling for example use in otherwise adverse conditions and longer shelf-life.

The following examples are provided for the purposes of illustration and are not intended to limit the scope of the invention.

EXAMPLE

This Example describes the production and analysis of a crystal and model of the present invention. It is to be noted that numbering of Fc-Ce3/Ce4 residues follows the convention of Dorrington et al, ibid.

The initiation of IgE-mediated allergic responses requires the binding of IgE antibody to its high affinity receptor, FcεRI. Crosslinking of FcεRI initiates an intracellular signal transduction cascade that triggers the release of mediators of the allergic response. The interaction of IgE-Fc domains with FcεRI is a key recognition event that is central to this process and mediated by the extracellular domains of the α-chain of FcεRI. This Example describes the solution of a crystal structure of the human IgE-Fc:FcεRIα complex, the coordinates of which are disclosed in Table 1. The crystal structure reveals that one receptor binds one IgE-Fc asymmetrically through interactions at two sites involving both N-terminal IgE-Fc Cε3 domains. The interaction of one receptor with IgE-Fc blocks the high-affinity binding of a second receptor and features of this interaction are conserved in other Fc receptor family members. The structural analysis suggests new approaches to the inhibition of IgE binding to FcεRI for the treatment of allergy and asthma.

A. Introduction

The high affinity IgE receptor (FcεRI) is found on the surface of effector cells of the immune system that initiate cellular reactions associated with the allergic response, anaphylaxis and anti-parasitic immunity[1,2]. The human receptor can form either a trimeric $\alpha\gamma_2$ or tetrameric $\alpha\beta\gamma_2$ structure on cell surfaces, with the extracellular domains of the α-chain conferring the ability to bind antibodies of the IgE class with high affinity ($K_D \sim 10^{-9}$-10^{-10}M). IgE antibodies bind to the receptor in the absence of antigen and thus the receptor adopts the antigenic specificity of the prevalent IgE repertoire. Crosslinking of the receptor through the engagement of antigen:antibody interactions leads to the initiation of a lyn and syk kinase-mediated signal transduction cascade, analogous to that induced by T and B cell receptors[3-5]. In mast cells, receptor activation leads to rapid degranulation and release of histamine followed by the synthesis and release of

prostaglandins, leukotrienes, cytokines and other mediators of the allergic response. Anti-parasitic responses can be triggered through a similar activation of eosinophils, leading to the release of granular proteins toxic to schistosomes and other parasites. FcεRI belongs to a family of antibody-binding receptors that also mediate interactions of soluble IgG and IgA antibodies with cells of the immune system[3,5]. IgG-Fc receptors regulate inflammation pathways, B cell development, and Natural Killer Cell activation and are therefore important in many aspects of immunity and disease.

Atopic diseases, such as allergy, asthma, and eczema, comprise a wide spectrum of pathologies associated with the inappropriate activation of the immune system to environmental antigens[6,7]. Dramatic increases in atopic disease have been observed in this century, particularly in developed countries. Allergic diseases have been associated with the IgE network through genetic studies in both mice and humans, suggesting a role for polymorphisms of the FcεRI β-chain and CD14 in atopic individuals[7,8]. The interaction of the IgE antibody with FcεRI is central to these immune reactions, providing an attractive target for the inhibition of all IgE-mediated allergic disease. Clinical studies of allergic individuals using anti-IgE monoclonal antibody therapy has demonstrated that this is a viable approach to disease treatment[9,10]. Further development of treatments for allergy, asthma and anaphylaxis, may benefit from structural insights into the IgE:FcεRI interaction.

A recent report disclosed the crystal structure of the human FcεRI α-chain ectodomains[11], which revealed a highly bent arrangement of two immunoglobulin domains. Four solvent-exposed tryptophans cluster at the top of the receptor, forming a large hydrophobic surface for potential interactions with the IgE-Fc. This tryptophan cluster borders the Fc binding-site mapped by mutagenesis studies, which implicate residues in the second domain of the receptor in IgE binding. The structural and functional data suggested that a large convex surface of the receptor could be involved in binding IgE, raising questions about the role of the tryptophans, the convex nature of the binding site and the mechanisms underlying the stoichiometry and binding specificity with IgE.

These questions are addressed with the solution of a crystal structure of a complex of the human IgE-Fc with FcεRIα as disclosed herein as well as of a crystal structure of the unbound IgE-Fc fragment as disclosed in 60/189,403, *ibid.* The structure of the complex reveals two interaction sites for the IgE-Fc on the receptor surface and clarifies how a 1:1 complex between antibody and receptor is formed. The two IgE-Fc Cε3 domains bind to distinct sites on the receptor; one is formed by the C-C' loop in the receptor D2 domain, while the second site involves the four solvent-exposed tryptophans. The IgE Cε4 domains do not form direct contacts with the receptor and point away from the Cε3 interaction sites. The structure of the complex accounts for previous mutagenesis and structural observations and shows that the Fc forms a complementary crown across the convex surface of the receptor. Comparison of the complex with the isolated IgE-Fc crystal structure suggests that large structural changes may occur upon IgE binding to its receptor (see 60/189,403, *ibid.*) The IgE-Fc:FcεRIα complex provides a model for understanding the function of other antibody Fc-receptors and new conceptual approaches to the inhibition of IgE-mediated diseases.

B. Structure determination of the complex

The crystallization of the IgE-Fc:FcεRIα complex required the expression of each protein using recombinant baculovirus technology. The expression of the FcεRIα was carried out essentially as described previously[11]. The IgE heavy chain contains four constant domains (Cε1-Cε4), in contrast to the three found in IgG antibodies. The interaction of FcεRI with IgE has been previously mapped to the two C-terminal constant domains of the IgE-Fc (domains Cε3/Cε4)[12-16]. The expression and purification of the human IgE-Fc Cε3/Cε4 domains was established as described (60/189,403, *ibid.*) and purified protein used to form complexes with FcεRIα. The best complex crystals (spacegroup $P42_12$) obtained with the wild type (wt) FcεRIα protein were small (~60-100μ/edge) and diffraction data was limited to a resolution of ~4.5 Å (Table 3, crystal form I). In order to improve the complex crystals, a triple carbohydrate mutant of FcεRIα (FcεRIαΔ4–6) was expressed in insect cells. The FcεRIαΔ4–6 mutant lacks carbohydrate at three of the seven native attachment sites (residues 74, 134, 140) and was previously shown to produce ~50% of the wt protein in CHO cells[17]. Complexes formed

with baculovirus-expressed FcεRIαΔ4–6 grow crystals in spacegroup R32 and diffract X-rays to a resolution of 3.25Å (Table 3, crystal form II). The structure was determined by molecular replacement techniques as described in Methods. Manual model building was done with the program O[18] and refinement carried out with CNS[19]. Current refinement statistics for the complex are shown in Table 3, with an overall R-free of 29.3% and R-cryst of 27.0% to 3.25Å. Fig. 1a shows electron density from a sigmaa-weighted 2Fo-Fc simulated annealing omit map calculated with the current model phases.

C. Overview of the complex

Both crystal forms of the IgE-Fc:FcεRIα complex contain a single 1:1 complex in the asymmetric unit, with similar overall geometric features (Fig. 1b, c). Given the low resolution of crystal form I, detailed interpretation of the interfaces is limited to crystal form II. Binding interactions are formed exclusively between the N-terminal Cε3 domains of the IgE-Fc with FcεRIα. The Cε4 domains of the IgE-Fc point away from the receptor structure and make no contacts with either receptor domain. The Cε3/Cε4 hinge regions are also not involved in direct receptor contacts. The two Cε3 domains are related by a nearly perfect diad axis (180.7°rotation), except for residues in the Cε2/Cε3-linker region (residues 331-336) (Fig. 1b, c). The Cε4 domains are also related by a nearly perfect diad axis (179.6° rotation), but the orientation of this axis differs from that determined for the Cε3 domains (Fig. 1b,c). The angle between the Cε3 and Cε4 domains also differs from that seen in the IgE-Fc alone (see 60/189,403, *ibid.*) While structured carbohydrate is visible in both the IgE-Fc and FcεRIα proteins, the carbohydrate groups do not contribute significantly to interactions between the two molecules. In addition, the IgE-Fc carbohydrate does not make any contacts across the IgE-Fc diad axis, but lies along the surface of each IgE-Fc domain.

The IgE-Cε3 domains bind at the top of the FcεRIα D1/D2 interface and along the backside of the D2 domain. The receptor contains two distinct binding sites for the two Cε3 domains. Site 1 refers to the interaction of one Cε3 domain exclusively with the C-C' region of the receptor D2 domain, as indicated, while Site 2 refers to the interaction of the second Cε3 domain with the top of the receptor at the D1/D2 interface (Fig. 1b,c). Site 1 is centered around Y131 on the C' loop in the receptor D2 domain.

Site 2 is located at the top of the receptor and involves four surface-exposed tryptophans (W87, W110, W113, and W156). The two chains of the Fc molecule bind the receptors using surface loops in Cε3 that are distal to the Cε4 domains. These loops are the immunoglobulin-fold BC (362-364), DE (394-395), and FG (424-427) loops, in addition to residues in the Cε2/Cε3-linker region near the interchain disulfide (328-336). The linker regions between the Cε2 and Cε3 domains are involved in interactions with the FcεRIα, which cause both linker segments to point up and away from the complex interface. The role of the IgE-Fc Cε4 domains is to provide a structural dimerization scaffold that enables two Cε3 domains to form the bivalent interaction with FcεRIα.

D. Structural basis for the formation of a 1:1 complex

Biophysical studies of the IgE-Fc:FcεRIα complex in solution indicate that a 1:1 complex is formed between the antibody and FcεRI[20-23]. This contrasts with models with a 2:1 stoichiometry that have been proposed for the interaction of the IgG antibody with the FcγRIIa and FcγRIIb receptors[24-26], as well as with the crystal structure of the MHC-class I like neonatal Fc receptor with IgG[27-29]. The observation of a 1:1 complex in both of the IgE-Fc:FcεRIα complex crystal forms is consistent with data on these complexes obtained using gel filtration and analytical ultracentrifugation techniques[22,23]. In principle, the 1:1 stoichiometry could arise due to FcεRI-induced conformational changes in the IgE-Fc, creating asymmetry in the Fc region, or by the binding of FcεRI across the Fc two-fold axis, creating a steric inhibition for the binding of a second receptor.

Fig. 2a and 2b show surface representations of the IgE-Fc:FcεRIα complex, demonstrating how the convex surface of the receptor interacts asymmetrically with the two IgE-Fc Cε3 domains. The receptor is positioned near the Fc-diad axis. There are two structural keys that dictate the formation of complexes with this stoichiometry: (1) The induction of structural asymmetry in the IgE-Fc Cε2/Cε3 linker and (2) Steric hindrance that blocks the binding of a second receptor.

Structural differences in the IgE-Fc domains are easily visualized by the superposition of the two Cε3 domains as shown in Fig. 2c. This superposition demonstrates that the Cε2/Cε3 linker regions comprised of residues 327-336, are

constrained to an asymmetric arrangement by interactions with FcεRI. Other loops that are involved in distinct interactions with the two FcεRI binding sites also adopt slightly different conformations in the two Cε3 domains, such as the FG loops indicated in Fig. 2c.

Binding of one receptor to sites 1 and 2 creates a steric block of the binding of a second receptor. Fig. 2d shows representations of the both the IgE-Fc and FcεRIα in which the complex has been separated to exposed the buried interaction surfaces. The Cε2/Cε3 linker amino acids form the top of an arch that conforms to the convex surface of FcεRIα, generating an asymmetric binding site for a single receptor. While some of the Cε3 binding surface remains accessible to the interaction with a second receptor, superposition of a second receptor onto the 1:1 complex shows significant steric overlap between receptors and the IgE-Fc Cε2/Cε3 linker amino acids. Thus the binding of one receptor effectively prevents the binding of a second due to both the asymmetric arrangement of the IgE-Fc Cε2/Cε3 linker and by receptor binding across the Fc diad axis. Both contribute sterically to interfering with the binding of a second receptor. Although different residues in the Fc are used to form sites 1 and 2, there are four residues (R334, G335, V336, and H424) common to both sites, providing direct interactions that prevent the simultaneous binding of two receptors to one IgE-Fc.

E. Structural changes in the receptor and IgE conformations upon binding.

The receptor shows little change in conformation upon complex formation with the Fc. The overall RMS difference in 158 Cα positions compared to the unbound receptor[11] is 1.11 Å. There are two loops on the receptor which adopt different conformations from those seen in the original FcεR1α structure[11], the BC loop in D1 (residues 30-35) and the C' strand in D2 (residues 127-133). The D2 C' strand is longer in the FcεR1α:IgE-Fc complex compared to the FcεR1α structure alone. In the receptor structure, the C strand forms hydrogen bonds to the C' strand through residue L127[11], while in the complex, the main chain hydrogen bonds extend to Y131. However, analysis of the FcεR1α structure in multiple crystal forms (Garman *et al.*, in preparation) shows that the C' strand can adopt a variety of conformations depending on the chemical

environment. The BC loop in Domain 1 also adopts different conformations in different crystal forms, but this region is not involved in IgE-Fc interactions.

The IgE-Fc in the complex is observed in a conformation that is very similar to the Fc domains of IgG antibodies[30,31]. Similar binding interactions between IgG antibodies and FcγRs could form an analogous 1:1 complex, as suggested by biophysical studies of the IgG-Fc interaction with FcγRIII[32]. In contrast to the similarities of the bound IgE-Fc to IgG-Fc structures, the crystal structure of the IgE-Fc alone shows a large re-arrangement of the two Cε3 domains that is greater than the conformational variation observed in IgG-Fc structures (see P_AL-9, *ibid.*). The IgE-Fc conformation may change substantially from the unbound conformation, which may exist in multiple conformational states that interact weakly with the receptor. This conformational variation in the IgE-Fc structure suggests new avenues to inhibiting IgE-receptor interactions using allosteric modulators that could stabilize the closed, unbound IgE-Fc structure.

F. Details of the binding surfaces of the FcR:IgE interaction

The surface areas of both the IgE-Fc and FcεRIα that are involved in binding are shown in Fig. 2d, forming a total buried surface of ~1890 Å^2. The IgE-Fc adopts a concave or crown-like configuration at the N-terminal ends of the two Cε3 domains that matches the convex shape of the receptor, with the top of the crown defined by the Cε2/Cε3 linker residues. The two Cε3 domains form two distinct sets of interactions with the receptor that involve an overlapping but non-identical set of IgE residues in each of these two sites. Of the fifteen FcεRIα residues that contact the IgE-Fc, seven are aromatic and five of these aromatic residues are surface exposed tryptophans. In contrast, of the nineteen IgE-Fc residues that contact the FcεRIα, none are aromatic. The large fraction of aromatic receptor residues that are involved in this interaction and the large buried surface area may both contribute to the stability of the complex (K_D ~ 10^{-9}–10^{-10} M).

Fig. 3a shows a plot of the IgE-Fc residues that are buried in the interaction with the receptor. Cε3 residues involved in Site 1 are in the top half of the plot and form specific interactions with FcεRIα residues shown in Fig. 3b. Nine amino acids from the

IgE and seven amino acids from the receptor form Site 1 (Fig. 3b and Fig. 4a), burying a total of ~835Å^2 of surface area. The IgE residues are from four distinct regions of the IgE-Fc sequence that are predominantly loop and adjacent strand residues, including the N-terminal linker (residues 334-336), the BC loop (residues 362-364), the DE loop (residues 394-395) and the FG loop (residue 424). The receptor residues derive from two regions of the D2 domain, involving the C strand (residues 117 and 119) and the flexible C'-E region (residues 126 and 129-132). Two potential salt bridges (αK117-Cε3D362 and αE132-Cε3R334) and 4 potential hydrogen bonds (αK117-Cε3G335, αY129-Cε3D362, αY131-Cε3D364 and αY131-Cε3H424) are formed across the Site 1 interface (Fig. 3b, Fig. 4a).

The Cε3 residues that are buried in the formation of Site 2 are shown in the bottom panel of Fig. 3a, Fig. 3c and in Fig. 4b. Residues R334, G335, V336, and H424 are buried in both Site 1 and Site 2 interfaces (Fig. 3a) but the remaining residues are unique to each of the two binding sites. Site 2 is larger than Site 1, with 10 amino acids from the IgE and 8 amino acids from the receptor forming a buried interface of 1040Å^2. The IgE residues are localized to two distinct regions of the sequence, including extensive interactions with the Cε2/Cε3-linker region (residues 332-336) and the FG loop (residues 424-427). The FcεRIα residues are from three regions of the sequence (Figs. 3c and 4b), the D1D2 linker region (residues 85-87), the BC loop (residues 110 and 113) and the FG loop (residues 156-158). Residues from the receptor D1 domain do not form direct interactions with the IgE-Fc, but are likely important for stabilizing the conformation of the D1D2 linker residues, including the highly conserved W87 (Figs. 3c and 4b). In contrast to the Site 1 interface, Site 2 contains primarily hydrophobic amino-acids with limited polar interactions. Site 2 involves 3 potential hydrogen bonds across the interface (αW156-Cε3G335, αQ157-Cε3N332 and αQ157-Cε3R334). The large amount of buried hydrophobic surface area may contribute to the high affinity binding constant.

G. Electron density appears for CHAPS detergent molecules in the Form II crystals.

One of these molecules sits above FcεRI-W156 and below the Cε3-FG loop near H424 in Site 2 (Fig. 3d). The position of the CHAPS heterocyclic core is analogous to

the position of the FcR C' loop residues in Site 1. Although the CHAPS interaction may be weak, this structure provides a foundation for using combinatorial synthetic chemistry methods to improve these initial binding interactions[33,34]. A high affinity inhibitor of the Site 1 interactions could prove to be a viable inhibitor of the IgE binding, given mutagenesis data that indicate the importance of this site in overall IgE:FcεRI affinity. In addition, H424, which is located next to the CHAPS binding site, makes contacts with the receptor in both Site 1 and Site 2. A small molecule inhibitor that could interact with both the Y131 pocket of Cε3 (site 1) and with H424 might effectively disrupt both Site 1 and Site 2 interactions with the receptor.

H. Locations of IgE and FcR mutations in the structure of the complex.

Mutagenesis studies of both the IgE-Fc and FcεRIα have been carried out in efforts to define the residues in both proteins that contribute to the stability of the complex. For FcεRIα, these studies have implicated residues located in the D2 domain, including amino acids 87, 113, 115, 117, 118, 120, 121, 122, 123, 128, 129, 130, 131, 132, 149, 153, 155, 156, 159, 160, 161[11,35-39]. While the general location of these residues is consistent with the observed complex, not all of the residues make direct contacts with the IgE-Fc, as shown in Figs. 4a and 4b. Of the residues identified by mutagenesis techniques, eight are observed to interact directly with the IgE (87, 113, 117, 129, 130, 131, 132, 156), twelve are within three residues that interact (115, 118, 120, 121, 122, 123, 128, 153, 155, 159, 160, 161) and the remaining amino acid (149) is buried and forms part of the hydrophobic core of D2.

The identification of the IgE-Fc binding site for receptor has implicated regions near the Cε2/Cε3 linker, the Cε3-AB helix and the Cε3-CD loop[12,15,16,40,41]. In general, most studies concur that the Cε2 and Cε4 domains do not interact directly with antibody. Residues in the IgE-Fc AB helix are likely to have an indirect effect on receptor binding, by altering the flexibility and geometry of the Cε3/Cε4 interface. Mutagenesis techniques have identified residues 333, 334, 376, 378, 380, 393, 414, 427 and 430 as possible contact residues in the IgE-Fc. Of these residues, three are observed as contact residues (333, 334, 427), one is within three residues (430) of a contact. However, four of these residues are located in the CD loop of Cε3 and are distant from

the IgE-Fc:FcεRIα interface (376, 378, 380, 414). Not all mutations at these residues are deleterious, for example R376A or R376K has little effect on binding, while R376E reduces the binding to receptor. Similarly, D409A, D409E or D409N are well tolerated, while D409R disrupts receptor binding. Thus it is possible that these selective mutations have an indirect effect on receptor binding, potentially through alterations in the conformation of the Cε3 domain.

I. The basis for IgE specificity and implications for other receptor:antibody complexes

Figs. 4a and 4b show schematic diagrams of the amino acid residues that lie within 4Å of each other in the Site 1 and Site 2 interfaces. Direct contacts are indicated by the connecting lines, which highlight residues that form the largest number of atomic contacts across the respective interfaces. Also shown are the residues that are found in the related human IgG receptors (FcγR1, FcγRII and FcγRIII, to the left) and in four subtypes of IgG antibodies (to the right).

In Site 1 there is little conservation of the residues that form the IgE-Fc:FcεRIα interface. Three residues are completely conserved (IgE residues 335, 362 and 394) in the Fc sequences, while there is poor conservation in the receptor sequences, except for the partial conservation of K117 and the relatively conserved Y129 (either Y or F). Interestingly, the conservation of K117 in three of the four receptors matches the complete conservation of D362 and G335, potentially preserving one of the two Site 1 salt bridges and one of the Site 1 hydrogen bonds. The conservative substitution of Y129 for F or Y in the IgG receptors also suggests that this site may be found in IgG-Fc complexes with the FcγRs. However, Y131, which forms a large number of atomic contacts across the interface and is buried in a shallow surface pocket on the IgE-Fc, is not conserved in the FcγRs (changing to either H or R). Given the central location of Y131 to the IgE interface, this residue may play an important role in immunoglobulin class specificity (Fig. 3b). For example, four of the five contact residues in IgE for Y131 are also different in the IgG-Fc sequences. In general, residues within the four IgG subtypes are highly conserved in the Site 1 interface (7/9 identical), as compared to the significant variation in the FcγR residues. Fig. 4b shows the conservation of interactions that are central to the Site 2 interface. P426 and L425 are absolutely conserved in all IgG

Fc sequences and P426 interacts with two absolutely conserved tryptophans in the FcεR complex (W87 and W110). The two tryptophans form a hydrophobic pocket on the surface of the receptor into which the proline inserts (Figs. 3c and 4c). Site 2 also includes three residues (IgE residues 332-334) that have been shown to affect binding of IgG subtypes to FcγRI. IgG1 binds with high affinity to FcγRI, whereas IgG2 does not, and the difference in binding affinity can be introduced into IgG1 by the substitution of residues LLG to PVA (IgE residues 332-334, highlighted in black in Fig. 4b)[42,43]. This region of the IgE-Fc interacts with the FcεRIα FG loop residues 156-158 (Figs. 3c and 4b). Previous mutagenesis experiments have also shown that the transfer of the FcεRIα FG loop to FcγRII confers detectable IgE binding[44]. Thus, residues involved in the formation of Site 2 are implicated in the binding and specificity of both IgE and IgG FcRs, consistent with a conserved binding mode across these members of the FcR family. Overall, five residues are completely conserved in these human receptors and IgG sequences that could form a common set of contacts. Variation in the FcγR FG loop sequences that contact the N-terminal linker region of the Fc fragment may provide key interactions that modulate the affinity of interaction of specific FcR:IgG pairs.

J. Conclusions

The crystal structure of the IgE-Fc:FcεRIα complex clarifies the atomic interactions that regulate the specificity and stoichiometry of protein:protein interactions underlying allergy and anaphylaxis. Similar complexes may form between IgG antibodes with their receptors, as suggested by previous mutagenesis studies and the structural analysis presented here, in contrast to models proposed for the interaction of IgG-Fc with the low affinity receptor, FcγRIIb[25] and FcγRIIa[24]. Knowledge of these interactions may allow the development of inhibitors for the treatments of allergy and asthma and may also facilitate the targeted engineering of therapeutic antibodies to interact with specific subsets of the FcR family[45].

The observed flexibility in the IgE Cε3/Cε4 hinge (see 60/189,403, *ibid.*) and the distinct interactions of the two Cε3 domains in Site 1 and Site 2, are consistent with a kinetic scheme for IgE binding shown in Fig. 5. In this scheme, the independent binding of each Cε3 domain in the FcεRIα complex, leads to two pathways for the full

dissociation of the complex. Surface plasmon resonance studies of IgE-Fc dissociation show two distinct kinetic dissociation rates that were hypothesized to represent the interaction of two different binding interactions between the IgE-Fc and FcεRIα, consistent with this kinetic scheme [16,41]. The IgE-Fc mutation R334S affects the biphasic dissociation kinetics of the IgE-Fc:FcεRIα complex by selectively accelerating the slow dissociation rate[16]. R334 is used in distinct and specific ways in Site 1 and Site 2, forming a salt bridge in Site 1 and van der Waals contacts in Site 2, consistent with the observation that one of these interactions could be more sensitive to the R334S mutation. The two dissociation pathways shown in Fig. 5 could exhibit two distinct overall kinetic rates that could be selectively affected by the R334S mutation. If the two Cε3 domains bind independently, with transient exposure of each site in the complex, inhibitors for either Site 1 or Site 2 could potentially accelerate the dissociation of receptor-bound IgE. Such inhibitors might prove useful in the treatment of acute allergic reactions in which dissociation of mast-cell associated IgE would be beneficial.

A model for the formation of a complex between an intact IgG antibody and Fc-receptor is shown in Fig. 6. In this model the crystal structure of the low affinity IgG receptor (FcγRIIb)[25] and one of the available intact IgG antibody structures (1IGY)[46] were superimposed on the IgE-Fc:FcεRIα complex. Superposition of the IgG structure is based on the Site 2 interactions, and this places the second IgG-Fc Cg2 domain within close proximity of the Site 1 binding surface without any conformational rearrangements (Fig. 6). The Fab arms of IgG are flexible and are also easily accommodated into this complex. Antigen-induced crosslinking of antibody:FcR complexes, leads to the co-localization of Fc receptors and the initiation of intracellular signal transduction cascades[2,47]. Within the one of the IgE-Fc:FcεRIα crystal forms and the IgE-Fc crystals (60/189,403, *ibid.*), Cε3 domains from adjacent molecules are observed to form packing interactions in the crystal through a strand to strand hydrogen-bonding interaction. Such interactions could potentially play a role in orienting crosslinked receptors, allowing the intracellular approach of receptor-associated kinases to adjacent γ-chain cytoplasmic tails, initiating the signal transduction cascade. A potential role for Cε3:Cε3 interactions in signal transduction remains to be tested.

K. Methods

1. Crystallization of the human IgE-Fc:FcεRIα complex

Human IgE-Fc Cε3/Cε4 domains and a carbohydrate mutant of the FcεRIα[11] were expressed in insect cells essentially as described for IgE-Fc Cε3/Cε4 in 60/189,403. Complexes of wt-Fc- Cε3/Cε4 and wt-FcεRIα produced only poorly diffracting crystals. Since the receptor is heavily glycosylated (~33% carbohydrate by weight), and the carbohydrate sites are dispersed on the receptor surface, a subset of these attachment sites was removed to improve the protein crystallization. A previously-described carbohydrate mutant of the receptor[17] lacking three of the seven wild type carbohydrate sites (residues 74, 135, and 140) located on both D1 and D2 in the receptor structure. The triple receptor mutant, FcεRIαΔ4-6 was subcloned into the pvl1392 baculovirus transfer vector and recombinant virus produced. The mutant receptor was active, expressed well and was purified by affinity chromatography similarly to the wt protein. Purified wt-Fc and αΔ4-6 or wt-α were incubated to form complex, which was subsequently purified by gel filtration chromatography using a Pharmacia Superdex 75 column and concentrated to 10 mgs/ml. Crystallizations were carried out using the the hanging drop method of vapor diffusion. Crystals of the wtIgE-Fc:wt-FcεRIα complex were grown from 1.4-1.6M Ammonium Sulfate, 100mM Tris pH 8.5, over a period of 8-12 months (Form I). Purified wtIgE-Fc:αΔ4-6 complex was crystallized using 100mM Tris, pH 8.5, 1.4-1.6M Ammonium Sulfate, and 8mM CHAPS at room temperature. Crystals were then moved into harvest buffer (Form I: 2.1-2.7M Ammonium Sulfate, 100mM Tris pH 8.5 or Form II: 1.6-2.0 M Ammonium Sulfate, 100mM Tris pH 8.5, and 0.8mM CHAPS). Crystals were frozen in harvest buffer supplemented with 15% glycerol. Data sets were collected at ALS 5.0.2 beamline and the APS DNDCAT 5-ID-B beamline at -160 C using an ADSC Quantum 4 detector or a MarCCD detector. Images were processed using the DENZO/SCALEPACK programs[48]. Form I crystals belong to spacegroup $P4_12_12$ with cell dimensions a=b=126Å, c=129Å and Form II crystals belong to the space group R32 with cell dimensions a=192.8Å and c=302.4Å (hexagonal setting). Intensities were adjusted using the TRUNCATE program prior to molecular replacement using the AMoRe[49] and EPMR programs[50].

2. Crystal structure determination and refinement

Molecular replacement for the Form II crystal was performed using coordinates from the 2.4Å structure of the receptor[11]. The use of normalized structure factors in AMoRe was critical to the success of the search. Both AMoRe and EPMR produced crystallographically equivalent locations for the receptor. 2Fo-Fc electron density maps with phases from the receptor revealed density corresponding to the two Cε3 portions of the Fc. A model for the core residues of Cε3 was created (see 60/189,403, *ibid.*) based upon homologous residues from an intact IgG structure 1IGT [46]. A new 2Fo-Fc map was created with phases from the receptor and core residues of Cε3. This map showed density for the locations of the two Cε4 domains. A model for the core residues in Cε4 was made based upon the homologous residues in 1IGT. Rigid body refinement of the receptor, the core residues in Cε3, and the core residues in Cε4 reduced the Rfree to 45%. 2Fo-Fc maps and composite omit maps revealed clear density for protein and carbohydrate atoms absent from the model. The Form I crystal structure was solved by molecular replacement using the complex model from Form II, with a clear top solution. Given the limited resolution of Form I, refinement was limited to rigid body minimization.

Refinement was continued with the 3.25Å Form II data using the CNS program[19]. Non-crystallographic symmetry restraints of 300 kcal/mol/Å^2 were imposed on all atoms in the Fc except the loops that interact with the receptor. Refinement was performed using all data from 40-3.25 Å with |F|>0 and using a bulk solvent correction. After inserting all the missing loops from the protein chains, CHAPS molecules were located as large peaks of positive density in Fo-Fc maps. The current refinement statistics are summarized in

5 Table 3. Figures were made using the programs Molscript[51] and Grasp[52].

Table 3. Data Collection and Refinement Statistics

	Data		
Data Set	Form I	Form II–Low Res.	Form II-High Res.
Resolution (Å) ‡	30-4.5 (4.66-4.5)	30.0-4.00 (4.14-4.00)	40.0-3.25 (3.37-3.25)
Source	APS DND 5ID	ALS 5.02	APS DND 5ID
Wavelength (Å)	1.0000	1.2000	1.0340
Completeness‡	99.5 (97.7)	99.7 (98.3)	99.7 (98.7)
Ave. Redundancy‡	7.0 (5.8)	5.0 (3.9)	3.7 (3.4)
Rmerge‡	17.8 (57.5)	15.2 (75.0)	12.4 (90.1)
I/sigI‡	5.9 (2.0)	4.4 (2.0)	13.3 (1.5)
observations (unique) ‡	39925 (5703)	91617 (18459)	125663 (34235)
# refl in refinement (free)		18455 (945)	34156 (1736)

		Refinement (Form II, 3.25Å)			
Rfactor/Rfree	Total # atoms	Protein	Carbohydrate	Detergent	Sulfate
25.8/28.1	5251	4821	259	146	25

RMSD		Average B			
Bonds	Angles	Overall	Receptor	Fc chain 1	Fc chain 2
0.0102	1.58	91.0	63.2	94.9	99.4

Ramachandran			
Favored	Allowed	Generous	Disallowed
77.0%	21.5%	1.5%	0.0%

‡ Last shell is shown in parentheses

$R_{merge}=\Sigma|I_i-<I>|/\Sigma|I|$, where I_i is the intensity of and individual reflection and <I> is the average intensity of that reflection.

$R_{cryst}= \Sigma||F_p|-|F_c||/\Sigma|F_p|$, where F_c is the calculated and F_p is the observed structure factor amplitude.

10

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While the various embodiments of the present invention have been described in detail, it is apparent that modifications and adaptations of those embodiments will occur to those skilled in the art. It is to be expressly understood, however, that such modifications are adaptations are within the scope of the present invention, as set forth in the following claims.